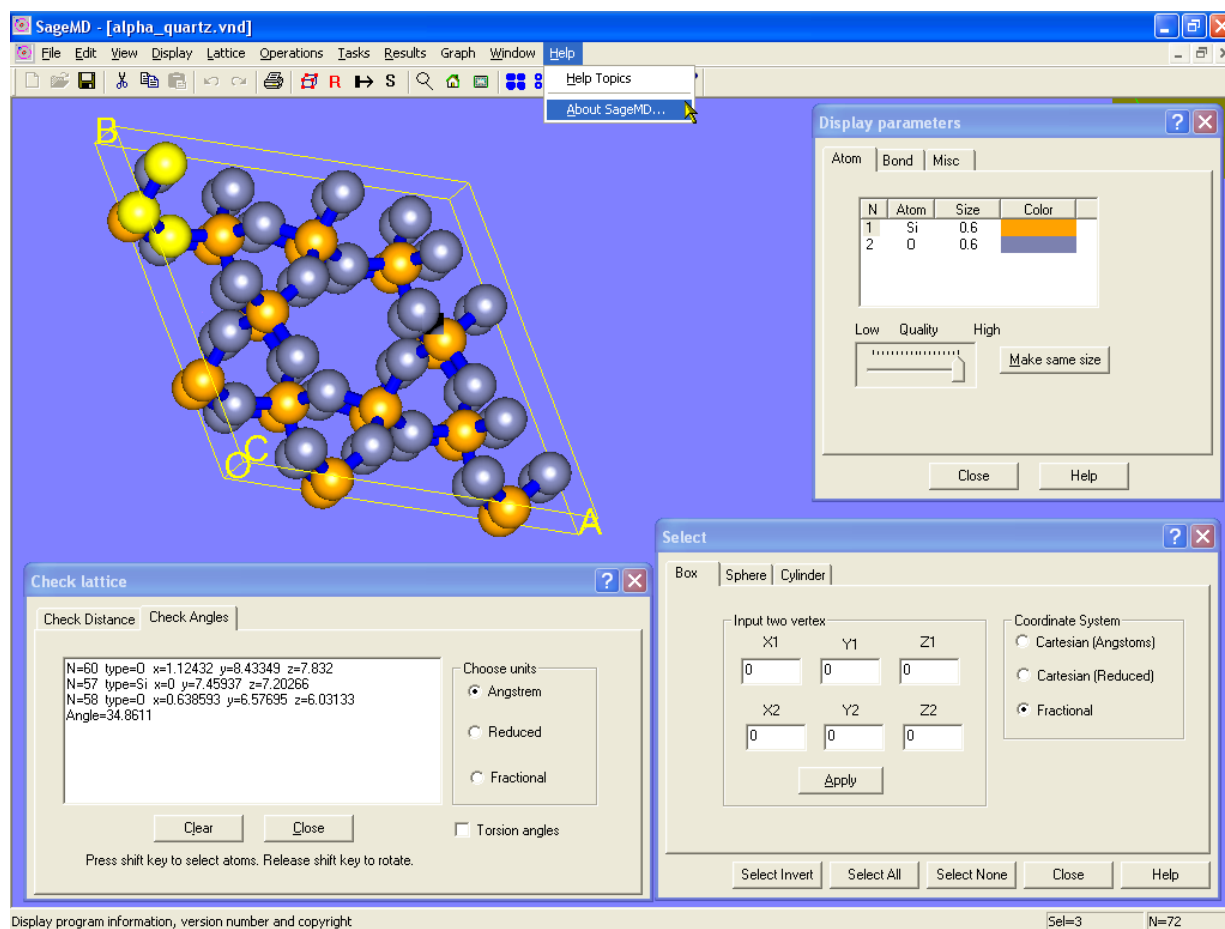


SageMD

User Manual



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Preface

Thank you for your choice of **SageMD**, the molecular dynamics simulation software allowing you to perform molecular dynamics (MD) calculations on your computer. We hope that you will find **SageMD** useful for your research, and this User Manual will help you to become familiar with this software.

This User Manual consists of 10 Chapters. Chapter 1 explains requirements for using **SageMD** and describes the procedures for its installing and uninstalling. Chapter 2 describes mainframe problems and methods, implemented in **SageMD**. Chapter 3 acquaints with software's Main Window Menus and ToolBar. The base dialog boxes itemize in Chapter 4. Chapter 5 explains how to prepare and execute molecular dynamic simulations with **SageMD**. Chapter 6 tells about libraries and databases used for prepare input data for MD simulation. The MD simulation of Al crystal melting is shown for example in Chapter 7. Chapter 8 describes the result files and documents. Chapter 9 explains how to work with 3D graphics. Chapter 10 answers the most possible user questions. The list of used literature is shown in References.

Notations, used in this Manual:

All names of menu items, dialog boxes, controls etc., denotes as underlined.

Example: Click the OK button.

All hyperlinks are accompanied by text references (in parentheses) to corresponding section. It makes this document convenient for work in both electronic and printed version.

Example: Use [Set potential](#) (4.14) dialog to set interatomic potential for atoms.

Warning: **SageMD** development is going on now, so some discrepancies between User Manual text and today software's state may take place. These discrepancies will have been eliminated in the next visions of the Manual.

1 Installation and hardware requirements

1.1 Minimum requirements

Computer	Intel Pentium II or compatible
Memory	128 MB RAM
Screen resolution	800x600
Color performance	16 bit (65536) colors
Operating system	Windows 98, Windows Me, Windows NT 4.0, Windows 2000 Professional, Windows XP

1.2 Installation

Locate the sagemd.exe file and run it. Follow the instructions on your screen.

1.3 Uninstalling

Click the "Start" button; select "Settings", then "Control Panel".

The Control panel will be displayed. Click the "Add/Remove Programs" icon.

Locate "**SageMD**" in the application list and click it. **SageMD** will be removed from your system.

2 Mainframe problems and methods, implemented in SageMD

2.1 About program

Molecular dynamics (MD) is widely used to study materials structure and properties based on the microscopic (atomic scale) models. The range of possible applications for MD simulation is very broad and is constantly growing with the advances in computer power and accessibility. Beside classical monographs (see, for example, refs. ^{1, 2, 3, 4}) that describe in detail the theoretical and algorithmic foundations of MD, there exist numerous applications and computer codes (see for example refs. ^{5, 6, 7}). The advent of massively parallel computers immensely expanded the range of possible applications of MD. It is currently feasible to study ensembles of $10^7 \div 10^8$ atoms/simple molecules with the MD approaches.

SageMD is specifically targeted at modeling materials with the wide range of chemical bonding situations, including metallic, covalent and ionic bonds. The goal was to make **SageMD** a multipurpose, flexible and user-friendly package easy to use in a typical computing environment. The major part of the code is written in FORTRAN 90, while some modules are written in MS VC++. Graphical User Interface (GUI) simplifies user interaction with the code and provides for setup of initial data via intuitive and easy to operate dialogues and menus. Initial data, results, parameters, MD cell, and crystal lattice can be inspected on the computer screen. User-friendly GUI also allows for analysis of results with a variety of graphs and tools. GUI gives the next main features:

- 3-D visualization of the periodic atomic structures.
- Copying, moving, deletion, and changing types of the highlighted atoms.
- Highlighting the crystal lattice fragments as boxes, spheres, and cylinders.
- Visualization of rotations and displacements.
- Calculations of bonds lengths and angles between atoms.
- Visualization of orthogonal and perspective projections.
- Exporting atom coordinates to .car, .fdf, .xtl, and .xyz file formats.
- Support for dynamic visualization of modeling results while calculations are running.

SageMD code can be used to model properties of materials at constant temperature and/or constant pressure, to study behavior of the crystal lattice under expansion or compression, to calculate Radial Distribution Function (RDF), and to derive atomic diffusion coefficients. The user can choose different boundary conditions, namely: periodical boundary conditions, free surfaces, and movable walls. In addition, the QEq approach for interatomic energy calculation, which takes into account atomic charge distribution, has been incorporated into **SageMD** code for modeling the properties of materials with covalent chemical bonds. For derivation of atomic charges and other parameters of force fields used in **SageMD**, quantum chemical programs (e.g. GAUSSIAN⁸, ABINIT⁹, and SIESTA¹⁰) have been used.

2.2 Molecular Dynamics. Some of the theory

2.2.1 Principles of MD simulation

In classical dynamics the motion is fully determined if a Hamiltonian is known for the system. Hamilton equations (1) determine the ensemble evolution^{11, 12}.

$$\begin{aligned}\frac{dq_i}{dt} &= \frac{\partial H(q, p)}{\partial p_i}, \\ \frac{dp_i}{dt} &= -\frac{\partial H(q, p)}{\partial q_i}, \quad i = 1, 2, \dots, N.\end{aligned}\tag{1}$$

For the ensemble of structureless particles interacting with each other via an effective potential that depends only on their mutual position, the generalized coordinates, and momenta, the Hamiltonian is determined by the following relations:

$$q_i \equiv r_i, \quad p_i \equiv m v_i, \quad H(r, p) = \sum_{i=1}^N \frac{p_i^2}{2m} + U(r),\tag{2}$$

where $U(r)$ is the total potential energy of the ensemble of particles under consideration. Note, $U(r)$ depends only on the spatial coordinates of the particles $r \equiv (r_1, r_2, \dots, r_N)$. Hence, the system of equations (1) is given by

$$\begin{aligned}\frac{dr_i}{dt} &= v_i, \\ m \frac{dv_i}{dt} &= -\frac{\partial U(r)}{\partial r_i}.\end{aligned}\tag{3}$$

By introducing the force that affects the particle with a number i , $F_i = -\frac{\partial U(r)}{\partial r_i}$, the system of equations (2) can be rewritten as:

$$\begin{aligned}\frac{dr_i}{dt} &= v_i, \\ m \frac{dv_i}{dt} &= F_i \quad i = 1, 2, \dots, N.\end{aligned}\tag{4}$$

For the additive pairwise interactions, the equations of motion are given by

$$\begin{aligned}\frac{dr_i}{dt} &= v_i, \\ m \frac{dv_i}{dt} &= \sum_{j \neq i} F_{ij}, \quad i = 1, 2, \dots, N,\end{aligned}\tag{5}$$

where F_{ij} is an interaction force between particles i and j .

Adiabatic approximation (the Born-Oppenheimer approximation¹³) further allows us to describe interatomic interactions via effective potentials.

The classic equation of motion (3) can be used to describe the state of microparticles (atoms and molecules) if $\lambda \ll a$, where λ is the de Broglie wavelength for a particle and a is the typical distance between particles. De Broglie's wavelength for the particle with the mass m ($m = \mu \cdot M_u$) is determined by the relation:

$$\lambda = \sqrt{\frac{2\pi \hbar^2}{\mu \cdot M_u \cdot kT}}. \quad (6)$$

Taking into account the values of the fundamental constants¹⁴ Planck constant, Boltzmann constant, and unit of atomic mass:

$\hbar = 1.0546 \cdot 10^{-34} \text{ J} \cdot \text{s}$, $k = 1.3807 \cdot 10^{-23} \text{ J} / \text{K}$, $M_u = 1.6605 \cdot 10^{-27} \text{ kg}$, for temperature $T \sim 300\text{K}$, the equation (6) can be written as:

$$\lambda \cong \frac{1}{\sqrt{\mu}}, \quad (7)$$

where μ is the atomic or molecular mass of the particle.

Table 1 contains calculated values of the relation λ/a for some metals and gases. For metals the value of a represents the interatomic interaction between the nearest neighbors in a crystal lattice under normal conditions. For gases the value of a is related to the σ parameter in the Lennard-Jones interparticle potential. The numerical values of parameters a and σ were taken from refs. ¹⁴ and ¹⁵.

Sub-stance	a , Å	Molecular or atomic mass, μ , g/mole	λ / a
C (dia- mond)	1.544	12.011	0.187
Al	2.863	26.981	$6.72 \cdot 10^{-2}$
Cu	2.556	63.546	$4.91 \cdot 10^{-2}$
W	2.741	183.85	$2.69 \cdot 10^{-2}$
Ar	3.418	39.948	$4.63 \cdot 10^{-2}$
N ₂	3.749	28.013	$5.034 \cdot 10^{-2}$
H ₂	2.968	2.016	0.237

Table 1. Numerical values of relation of the de Broglie wave length to the typical interatomic distance.

As can be seen from the results given in Table 1, the expression $\lambda/a \ll 1$ is satisfied for metals. At the room and higher temperatures this condition is also satisfied for many gases.

The trajectories and velocities of particles calculated by solving equations (3) provide information about the thermodynamic and kinetic properties of a substance. The thermodynamic parameters of a substance (macroscopic parameters) in the classical statistical physics are determined from mean ensemble values of the respective dynamic functions, $A_{\text{obs.}} = \langle A \rangle$. Symbol $\langle \dots \rangle$ denotes the ensemble averaging for the dynamic function $A(q, p)$ with respect to coordinates and momenta. The ergodic hypothesis¹⁶ is used to calculate $A_{\text{obs.}}$ from the velocities and trajectories:

$$\langle A \rangle = \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t A[v(\tau), r(\tau)] d\tau \quad (8)$$

2.2.2 Approaches to numerical solution of the equations of motion

There are several established methods for numerical solution of equations of motion in molecular dynamics. We will describe the ones implemented in the SAGE MD code. One of the early methods for numerical solution of the equations of motion in MD simulations was the Ver-

let method^{17, 18} for which the difference equations for the particle coordinates and velocities are given by:

$$\begin{aligned} r(t + \Delta t) &= 2r(t) - r(t - \Delta t) + a(t) \cdot (\Delta t)^2, \\ v(t) &= [r(t + \Delta t) - r(t - \Delta t)] / 2\Delta t. \end{aligned} \quad (9)$$

In terms of computer time and memory, the most effective method is the ‘leap-frog’ approach¹. The difference equations are given here by:

$$\begin{aligned} v(t + 0.5\Delta t) &= v(t - 0.5\Delta t) + a(t) \cdot \Delta t, \\ r(t + \Delta t) &= r(t) + v(t + 0.5\Delta t) \cdot \Delta t. \end{aligned} \quad (10)$$

The particle velocities at time t can be calculated from the equation

$$v(t) = [v(t + 0.5\Delta t) + v(t - 0.5\Delta t)] / 2. \quad (11)$$

*Velocity Verlet method*¹⁹ was also derived. It allows the calculation of coordinates and particle velocities in one time step. The difference equations for this case are given by:

$$\begin{aligned} r(t + \Delta t) &= r(t) + v(t) \cdot \Delta t + 0.5 \cdot a(t) \cdot (\Delta t)^2, \\ v(t + \Delta t) &= v(t) + 0.5 \cdot [a(t) + a(t + \Delta t)] \cdot \Delta t. \end{aligned} \quad (12)$$

This approach, however, requires that acceleration vectors for two time steps are stored in the computer memory. **SageMD** code uses this approach¹ to calculate the velocity vector. The velocity vector is calculated in two steps. At first the intermediate value of velocity is calculated

$$v(t + 0.5\Delta t) = v(t) + 0.5 \cdot a(t) \cdot \Delta t, \quad (13)$$

and, at the second step, the new acceleration vector $a(t + \Delta t)$ is calculated and stored in the computer memory utilizing the already unneeded array, which was freed after previously storing the acceleration vector $a(t)$. Subsequently, velocity values at the time moment $t + \Delta t$ are calculated from equation:

$$v(t + \Delta t) = v(t + 0.5\Delta t) + 0.5 \cdot a(t + \Delta t) \cdot \Delta t. \quad (14)$$

The total size of the arrays necessary to implement this algorithm is $9 \cdot N$, where N is the number of particles. To calculate the amount of required computer memory it is necessary to multiply this number by the number by the size of the computer word. In **SageMD** these arrays are of type double precision type, i.e. each array element takes 8 bytes. The main advantage of this algorithm is that particle coordinates and velocities are calculated at the same time step. This method, like all methods considered here, is the second-order method. The Gear and Beeman algorithms¹ are also implemented in the **SageMD** code for numerical solution of the equations of motion.

2.2.3 Optimal choice of the method to integrate equations of motion

The most accurate of the above integration methods is the Gear method. However, it requires a large amount of computer memory. The testing done for integration methods showed that the Gear method gives the lowest fluctuations of the total energy as compared to the other two methods. However, to hold the total energy at constant value, the size of the integration step

needs to be smaller than for Verlet or Beeman approach. This leads to the increase of computer time needed to conduct the MD simulation. The fluctuations of the total energy in the Beeman method are much smaller than in the Verlet method, while the requirements to the integration step are almost the same. However, Beeman method requires more computer memory. Since the major part of computer time is spent in step where forces are calculated, these methods can be considered equivalent with respect to computation rate. While Verlet method requires the least amount of computer memory compared to the other two methods, it causes appreciably larger fluctuations of the total energy. In **SageMD** code the *velocity Verlet* method is used as a default. Irrespectively of the integration method, however, it is necessary to make sure that the total energy of the system is preserved, or otherwise reduce the integration step. The 'integrator' command is implemented in the code to select the integration method.

2.2.4 MD simulation at constant temperature and constant pressure

The method suggested by Berendsen²⁰ is implemented in **SageMD** code for simulation at constant temperature and constant pressure. Temperature control in this approach is achieved by multiplying atom velocities by a coefficient λ , defined by the following equation:

$$\lambda = \left[1 + \frac{\Delta t}{\tau} \cdot (T_0 / T - 1) \right]^{1/2}, \quad (15)$$

where Δt is the integration time step, τ is the typical relaxation time, T is the current temperature and T_0 is the defined fixed temperature.

The pressure is controlled by changing atom coordinates and the size of the MD box. At every time step atom coordinates and the size of MD box are rescaled by the coefficient μ calculated from the expression:

$$\mu = \left[1 - \frac{\Delta t}{B \cdot \tau} \cdot (P_0 - P) \right]^{1/3}, \quad (16)$$

where Δt is the integration time step, τ is the relaxation time, P_0 is the pressure to be maintained constant, P is the current pressure value in the ensemble of particles and B is the compression bulk modulus. The value of the bulk modulus B need not be precisely equal to the real value. In **SageMD** this method is extended to account for the anisotropic case. The size of MD box can be therefore changed independently in three directions, and in general case the three components of the pressure tensor P_{xx} , P_{yy} , P_{zz} are specified instead of pressure of the scalar P_0 . In this case $P_0 = (P_{xx} + P_{yy} + P_{zz})/3$.

2.3 Interatomic Potentials

2.3.1 Pair Potentials

The choice and derivation of interatomic potential parameters is a central problem in molecular dynamic simulation. The non-empirical intermolecular and interatomic interaction potentials can be developed from the quantum-mechanical theory. The interatomic interaction is determined by the solution of the Schrödinger equation for a system of interacting nuclei and electrons. For the multi-particle system the Schrödinger equation can only be solved approximately. Important simplification is achieved by separating electronic and nuclear motions via adiabatic approximation¹³. The approximate solution of the Schrödinger equation provides the adiabatic

potential for nuclei. This potential is often sufficiently accurate and yields quality values for properties expressing interaction between atoms and molecules. De novo calculation of the potential for the many-electron system is, however, a complex problem. Therefore semi-empirical approaches, which contain parameters fitted to the experimental data, are often used in practice.

Due to proximity of atoms in the condensed matter under normal conditions, it is almost impossible to derive potentials for two-particle interactions from experimental data. Potentials, in fact, are not the pair potentials but represent effective potentials, which include effects of many-particle interactions²¹. These effective potentials are widely used to study properties of liquids and solids. Such potentials, fitted over a number of experimentally measured characteristics, allow us to calculate (quantitatively or semi-quantitatively) many important crystal properties. The equation of state, crystal elasticity modulus, adhesion energy, and the crystal structure are the examples of data used for fitting the parameters that enter effective potentials.

The types of interatomic pair potentials that are incorporated in the SAGE MD code are described below.

Lennard-Jones potential:

$$U(r) = \frac{U_0}{n-m} \cdot \left[m \cdot \left(\frac{r_0}{r} \right)^n - n \cdot \left(\frac{r_0}{r} \right)^m \right], \quad (17)$$

Morse and Morse modified potential:

$$U(r) = U_0 \cdot [\exp(-2\alpha \cdot (r - r_0)) - 2 \exp(-\alpha \cdot (r - r_0))] , \quad (18)$$

$$U(r) = \frac{U_0}{m-1} \cdot [\exp(-m\alpha \cdot (r - r_0)) - m \cdot \exp(-\alpha \cdot (r - r_0))] , \quad (19)$$

Buckingham and Buckingham modified potential:

$$U(r) = \frac{U_0}{1-6/\alpha} \cdot \left[\frac{6}{\alpha} \cdot \exp\left(-\alpha \cdot \left(\frac{r}{r_0} - 1\right)\right) - \left(\frac{r_0}{r}\right)^6 \right], \quad (20)$$

$$U(r) = \frac{U_0}{1-n/\alpha} \cdot \left[\frac{n}{\alpha} \cdot \exp\left(-\alpha \cdot \left(\frac{r}{r_0} - 1\right)\right) - \left(\frac{r_0}{r}\right)^n \right], \quad (21)$$

where U_0 is the minimum value of the potential, r_0 represents the interatomic distance when $U=U_0$, and n, m, α are additional potential parameters derived from theory or experiment.

Parameters for pair potentials are often derived by fitting the calculated lattice energy at zero temperature to the crystal sublimation energy, and by optimizing unit cell parameters and compressibility so they follow experimental data.

The constant temperature metal compression curves are also used for parameter fitting in the pairwise potentials. Currently the interatomic potential parameters for 26 metals representing different types of crystal lattices (body-centered, face-centered, hexagonal closed – packed) are incorporated in the code. Several different properties of metals are quite well reproduced by using these pair potentials, as shown in the recent contributions coming from our group^{22, 23, 24}.

To better represent Coulomb interatomic interactions, the use of variable atomic charges (reflecting changing atom configurations) has been suggested²⁵. The values of charges are computed with the charge equilibration (QEq) method²⁶ and the short-term interactions are approximated by the two-particle Morse potential. This approach was successfully applied to the simulation of the structure and properties of silicon oxide with four (quartz) and six (stishovite) coordinated silicon, amorphous silicon oxide, and transition of quartz to stishovite. The (QEq) method

has been incorporated in **SageMD** with potential parameters available for the number of ionic species. The Ewald summation is used to calculate the Coulomb interaction energy to avoid problems with necessary cutoff distances for these long-range interactions.

2.3.2 Many body potentials

The many body interaction potentials are different from the pair potentials as the total interaction energy of the system is not just a sum of all pair interactions. There are three main approaches to express the many body interactions²⁷: cluster, cluster functional potentials, and embedded atom method.

In 1985 paper Stillinger and Weber suggested the potential with two- and three-particle terms for modeling the diamond structure of silicon²⁸. The work describes a special case of the general expression for the potential interaction energy of N identical particles:

$$\Phi(1, \dots, N) = \sum_i v_1(i) + \sum_{\substack{i,j \\ i < j}} v_2(i, j) + \sum_{\substack{i,j,k \\ i < j < k}} v_3(i, j, k) + \dots + v_N(1, \dots, N) \quad (22)$$

The potential v_1 in this expression is responsible for modeling external forces. The expressions for v_2 and v_3 are given by

$$v_2(r_{ij}) = \varepsilon f_2(r_{ij}/\sigma), \quad (23)$$

$$v_3(r_i, r_j, r_k) = \varepsilon f_3(r_i/\sigma, r_j/\sigma, r_k/\sigma), \quad (24)$$

where ε and σ are introduced here in order to make the potential and the interatomic distance dimensionless. The following five-parameter function is used for the pairwise term of the potential:

$$f_2(r) = \begin{cases} A(Br^{-p} - r^{-q}) \exp\left(\frac{1}{r-a}\right), & r < a \\ 0, & r \geq a \end{cases} \quad (25)$$

This function is continuous and has continuous derivatives for all orders at point a . It is a useful feature for many MD-calculations that potential and all its derivatives are smooth functions with respect to coordinates of atoms. The three particle interactions are calculated from the following formula:

$$f_3(r_i, r_j, r_k) = h(r_{ij}, r_{ik}, \theta_{jik}) + h(r_{ji}, r_{jk}, \theta_{ijk}) + h(r_{ki}, r_{kj}, \theta_{ikj}), \quad (26)$$

$$h(r_{ij}, r_{ik}, \theta_{jik}) = \lambda \exp\left(\frac{\gamma}{r_{ij}-a} + \frac{\gamma}{r_{ik}-a}\right) \left(\cos(\theta_{jik}) + \frac{1}{3}\right)^2, \quad (27)$$

where θ_{jik} is the angle between r_{ij} and r_{ik} vectors; λ and γ are the potential parameters. The function h is calculated when the vector lengths (both r_{ij} and r_{ik}) are smaller than the cutoff radius a , and it is equal to zero otherwise. The potential parameters for silicon obtained from the ref.²⁸ are given below:

A	7.049556277
B	0.6022245584
p	4
q	0
a	1.8
λ	21.0
γ	1.2
σ	2.0951 \AA
ε	2.167374937 eV

Stillinger and Weber²⁸ conducted molecular dynamic calculations to model the silicon properties, in particular, silicon melting temperature. The potential, which they suggested, provides good description of the crystal silicon but it cannot be applied to the non-tetrahedral crystals formed at high pressures. Moreover, this approach was unable to provide an accurate estimate of the phase transfer temperature and the crystal cohesive energy when used with the single common set of parameters.

In the cluster functional method, the interaction energy is represented as:

$$\Phi = \sum_{i>j} \Phi_n(i, j; k \in a_n). \quad (28)$$

Each pair of interacting particles i, j is considered a part of the cluster a_n composed of n particles. The cluster configuration depends on the molecular structure. Interaction energy between two particles i and j depends not only upon their own coordinates but also on the coordinates of all $n-2$ particles in the a_n cluster. Tersoff potential is a typical example of a potential based on the cluster functional method.

The many-particle potentials suggested by Tersoff^{29, 30} are widely used for modeling silicon and other covalent materials. Here, the energy is calculated as a sum of pseudo-pair interactions with the attraction term being dependent on the local environment of the atom via the bond order factor:

$$E = \sum_i E_i = \frac{1}{2} \sum_{i \neq j} V_{ij} \quad (29)$$

$$V_{ij} = f_C(r_{ij}) \{a_{ij} f_R(r_{ij}) + b_{ij} f_A(r_{ij})\}. \quad (30)$$

where E is the total energy consisting of individual pair contributions, V_{ij} . The repulsive $f_R(r)$ and the attractive $f_A(r)$ forces are approximated by exponential functions, similar to the Morse potential:

$$f_R(r) = A \exp(-\lambda_1 r), \quad (31)$$

$$f_A(r) = -B \exp(-\lambda_2 r), \quad (32)$$

$$f_C(r) = \begin{cases} 1, & r < R - D, \\ \frac{1}{2} - \frac{1}{2} \sin\left[\frac{\pi}{2}(r - R)/D\right], & R - D < r < R + D, \\ 0, & r > R + D. \end{cases} \quad (33)$$

Function $f_C(r)$ confines the interactions to be within the “atomic radius”, which greatly reduces computational effort.

Bond order parameters, a_{ij} and b_{ij} , are the monotonic functions of the coordination number of atoms and depend on the valence angle (θ_{ijk}) with the neighboring atoms²⁹:

$$\begin{aligned} a_{ij} &= (1 + \alpha^n \eta_{ij}^n)^{-1/2n}, \\ \eta_{ij} &= \sum_{k(\neq i, j)} f_C(r_{ik}) \exp\{\lambda_3^3 (r_{ij} - r_{ik})^3\}, \\ b_{ij} &= (1 + \beta^n \zeta_{ij}^n)^{-1/2n}, \\ \zeta_{ij} &= \sum_{k(\neq i, j)} f_C(r_{ik}) g(\theta_{ijk}) \exp\{\lambda_3^3 (r_{ij} - r_{ik})^3\}, \end{aligned} \quad (34)$$

$$g(\theta) = 1 + c^2 / d^2 - c^2 / \{d^2 + (h - \cos \theta)^2\}.$$

Tersoff potential works for a wider range of modeling needs than the potential introduced earlier by Stillinger and Weber²⁸. This does not, however, come without a price. Tersoff potential is difficult to parameterize in the complex angular part and generally suffers from the large number of empirical parameters needed. The table below lists two sets of potential parameters for Si as suggested by Tersoff: version A provides a better description of surface properties, while version B models better elastic properties.

Table 2. Numerical values of the Tersoff potential parameters

	Si(A)	Si(B)
$A(eV)$	3.2647×10^3	1.8308×10^3
$B(eV)$	9.5373×10^1	4.7118×10^2
$\lambda_1 \begin{pmatrix} 0 \\ A^{-1} \end{pmatrix}$	3.2394	2.4799
$\lambda_1 \begin{pmatrix} 0 \\ A^{-1} \end{pmatrix}$	1.3258	1.7322
α	0.0	0.0
β	₁ 3.3675×10^{-1}	₆ 1.0999×10^{-1}
n	2.2956×10^1	₁ 7.8734×10^{-1}
c	4.8381	1.0039×10^5
d	2.0417	1.6218×10^1
n	0.0000	⁻ 5.9826×10^{-1}
$\lambda_3 \begin{pmatrix} 0 \\ A^{-1} \end{pmatrix}$	1.3258	1.7322
$R \begin{pmatrix} 0 \\ A \end{pmatrix}$	3.0	2.85
$D \begin{pmatrix} 0 \\ A \end{pmatrix}$	0.2	0.15

SageMD also incorporates the modifications of the Stillinger-Weber potential as suggested by Watanabe et al³¹. These are used to model properties of silicon, silicon oxide, and the interface between these materials. These potential parameters were obtained from quantum-chemical calculations.

In the embedded atom method (EAM) total energy is represented as follows³²:

$$\Phi = \sum_{i>j} \Phi_2(r_i, r_j) + \sum_i F(\rho_i), \quad (35)$$

where Φ_2 is the pair interatomic interaction energy,

$F(\rho_i)$ is the energy of atom i embedded in the environment with the electron density ρ_i created by the electrons of all other atoms of the system and considered to be additive:

$$\rho_i = \sum_{j \neq i} \rho(r_{ij}). \quad (36)$$

Here, $\rho(r)$ is the density of electrons in the atom at the distance r from the nucleus. The function $\rho(r)$ for the given element is derived either from quantum-chemical calculations or from empirical information. Functions $\Phi(r_i, r_j)$ and $F(\rho)$ are selected such as to obtain agreement of calculated values with experimental data for a crystal (lattice constant, elastic constants, sublimation energy, and the vacancy formation energy). The following functional form of $F(\rho)$ is universally used for all metals:

$$F(\rho) = -c\rho^{1/2}. \quad (37)$$

It allows one to interpret the $\rho(r)$ as an overlap integral of wave functions of atoms i and j . The embedded atom method is successfully used to study structures of metals and alloys, as well as investigation of crystal lattice defects, surface structures, etc. The (EAM) method in SAGE MD was extended for 23 elements³³.

2.3.3 EAM potential file format

The example of the EAM potential file is shown below. This format is similar to one used XMD code (<http://www.ims.uconn.edu/centers/simul/#xmd>).

```
# Johnson's potential for Au *
# cutoff = 5.700 A      *

#Time step determined for fcc Au, 200K (P. Chantrenne)
#DTIME=1.28e-14 s
#Lattice constant 4.08 A.

eunit eV

PAIR 1 1 3000 1 5.7000
1.529143e+02 1.520779e+02 1.512460e+02
1.504188e+02 1.495960e+02 1.487778e+02
1.479640e+02 1.471547e+02 1.463498e+02
...
DENS 1 3000 1 5.7000
5.041442e+01 5.025043e+01 5.008697e+01
4.992404e+01 4.976164e+01 4.959977e+01
4.943842e+01 4.927760e+01 4.911731e+01
...
EMBED 1 400 0 40
0.000000
-0.090532
-0.179980
...
```

Lines beginning with the sign (#) are comments and must be placed at the beginning of the file.

The "eunit" command sets energy units for the potential. It can be eV, K and erg. If this command do not present in the file, the energy units are eV.

PAIR type1 type2 table_size distance1 distance2

The pair or PAIR command identifies the table below as a pair potential function. The type1 and type2 are the atom types involved in the interaction.

The table_size is the number of points in the pair potential tables.

The distance1 and distance2 define the distance range in the angstrom units. The distance2 is the cutoff radius for the potential.

In the example above the pair table has distances from 1 to 5.7 angstroms.

The first value in the pair table corresponds the 1 angstrom of atoms separation.

The last value corresponds the cutoff distance (5.7 angstroms).

After the "pair" line is the pair potential table.

The number of values in the table must match the number specified in the "pair" line. The values must be separated by spaces or the new line characters.

DENS type table_size distance1 distance2

The DENS or dens command identifies the table below as a electron density function. The type specifies to which atom type the table belongs. The other parameters the same as in the pair line.

EMBED type table_size ro1 ro2

The EMBED or embed command identifies the table below as the embedded energy functions.

The ro1 and ro2 define the electron density range.

The first value of the table corresponds the ro1 value of the density, the last value of the table corresponds the ro2 value.

If the structure contains 2 different atom types you must prepare 3 files. The example of these files is below. (NiAl alloy)

The nial_ni_ni.pot file.

eunit K

```
PAIR 1 1 3000 1.000000 4.789502
0.000000E+00 9.146377E+05 9.097009E+05 9.047881E+05
8.998996E+05 8.950352E+05 8.901946E+05 8.853778E+05
8.805849E+05 8.758153E+05 8.710694E+05 8.663468E+05
...
DENS 1 3000 1.000000 4.789501
0.000000E+00 3.775296E-25 3.770337E-25 3.765355E-25
3.760348E-25 3.755318E-25 3.750264E-25 3.745187E-25
3.740086E-25 3.734963E-25 3.729817E-25 3.724649E-25
...
EMBED 1 2362 0.0000000 1.705184e-24
-1.137440E-13 -7.041029E+02 -9.087178E+02 -1.037061E+03
-1.127587E+03 -1.194739E+03 -1.245699E+03 -1.284611E+03
-1.314099E+03 -1.335936E+03 -1.351383E+03 -1.361368E+03
...
```

The nial_ni_al.pot file.

eunit K

```
PAIR 1 2 3000 1.100000 5.463932
6.850880E+05 5.270333E+05 5.237156E+05 5.204156E+05
5.171331E+05 5.138681E+05 5.106205E+05 5.073902E+05
5.041770E+05 5.009810E+05 4.978020E+05 4.946400E+05
...
```

The nial_al_al.pot file.

```

eunit K
PAIR  2 2 3000 1.000000 5.554982
0.000000E+00 7.524923E+05 7.480864E+05 7.437026E+05
7.393409E+05 7.350010E+05 7.306829E+05 7.263866E+05
7.221119E+05 7.178585E+05 7.136267E+05 7.094161E+05
...
DENS  2 3000 1.000000 5.554981
4.567510E-11 4.321021E-25 4.317819E-25 4.314566E-25
4.311262E-25 4.307906E-25 4.304500E-25 4.301044E-25
4.297538E-25 4.293982E-25 4.290377E-25 4.286722E-25
...
EMBED  2 2213 0.000000 2.054483e-24
-8.057838E-14 -5.634532E+02 -5.423222E+02 -4.451216E+02
-3.138738E+02 -1.632606E+02 -1.056015E-01 1.718979E+02
3.505433E+02 5.344154E+02 7.225567E+02 9.142900E+02
...

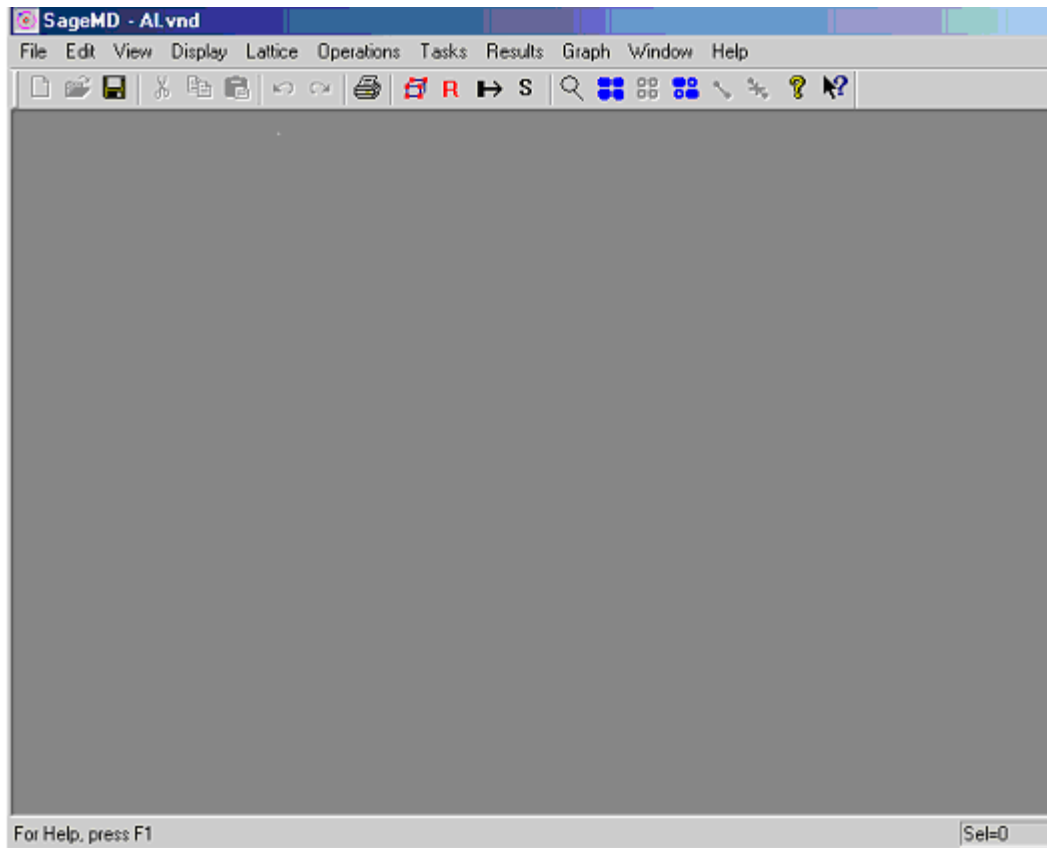
```

Note that nial_ni_al.pot file contains only the pair interaction table. The other examples of the EAM potentials you can find in the EAM subdirectory of the SageMD installation directory.

3 The Basic Operations of SageMD Main Window

3.1 Starting SageMD. Main Window

Click the Start button, move the mouse pointer sequentially to Programs then to **SageMD**, and click **SageMD**. **SageMD** will start and the **SageMD** main window will be displayed.



Alternative method – from My Computer or Windows Explorer, double-click **SageMD**

icon  .

3.2 SageMD main window menus

3.2.1 File menu

<u>N</u> ew	Ctrl+N
<u>O</u> pen...	Ctrl+O
<u>C</u> lose	
<u>S</u> ave	Ctrl+S
Save <u>A</u> s...	
<hr/>	
<u>E</u> xport...	
<u>I</u> mport...	
ConvTo <u>U</u> nix...	
<hr/>	
<u>P</u> rint...	Ctrl+P
Print <u>P</u> review	
Print <u>S</u> etup...	
<hr/>	
Recent Files	
<hr/>	
<u>E</u> xit	

The File menu offers the following commands:

New	Creates a new document.
Open	Opens an existing document.
Close	Closes an opened document.
Save	Saves an opened document using the same file name.
Save As	Saves an opened document to a specified file name.
Export	Saves an opened document to a specified file format.
Import	Opens a document using a specified file format.
ConvToUnix	Converts a WIN/DOS text file to a Unix text file format.
Print	Prints a document.
Print Preview	Displays the document on the screen, as it would appear printed.
Print Setup	Selects a printer and printer connection.
Exit	Exits SageMD

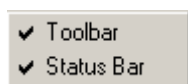
3.2.2 Edit menu

<u>U</u> ndo	Ctrl+Z
<u>R</u> edo	Ctrl+Y
<hr/>	
<u>C</u> ut	Ctrl+X
<u>C</u> opy	Ctrl+C
<u>P</u> aste	Ctrl+V
<hr/>	
Capture <u>w</u> indow	
Capture <u>i</u> mage	
Capture image to <u>f</u> ile	

The Edit menu offers the following commands:

Undo	Reverse previous editing operation.
Redo	Reverse previous undo command action.
Cut	Deletes data from the document and moves it to the clipboard.
Copy	Copies data from the document to the clipboard.
Paste	Pastes data from the clipboard into the document.
Capture window	Copies the SageMD screen onto the clipboard. After that you can paste the image into the documents of the other applications.
Capture image	Copies the any part of the SageMD screen to the clipboard. To do it hold the left mouse button and move mouse to draw the rectangle. After releasing the mouse button the part of the screen that lies inside the rectangle will be copied to the clipboard. After that you can paste the image into the documents of the other applications.
Capture image to file	Copies the any part of the SageMD screen to the bitmap file. To do it hold the left mouse button and move mouse to draw the rectangle to select the part of the screen to save. After releasing the mouse button the standard Save as dialog will be displayed. Use it to save the image into the file.

3.2.3 View menu



The View menu offers the following menu items:

3.2.3.1 Toolbar menu item

Use this command to display and hide the [Toolbar](#) (3.3), which includes buttons for some of the most common commands in **SageMD**. A check mark appears next to the menu item when the Toolbar is displayed.

3.2.3.2 Status Bar menu item

Use this command to display or hide the Status Bar, which describes the action to be executed by the selected menu item or pressed toolbar button. A check mark appears next to the menu item when the Status Bar is displayed.

The status bar is displayed at the bottom of the **SageMD** window. To display or hide the status bar, use the Status Bar command in the View menu.

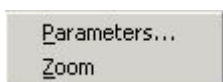
The left area of the status bar describes actions of menu items as you use the arrow keys to navigate through menus. This area similarly shows messages that describe the actions of toolbar buttons as you depress them, before releasing them. If after viewing the description of the toolbar button command you wish not to execute the command, then release the mouse button while the pointer is off the toolbar button.

The right areas of the status bar indicate the following:

Sel= The number of the currently selected atoms.

N= The number of atoms in the lattice

3.2.4 Display menu



The Display menu offers the menu items:

3.2.4.1 Parameters menu item


Parameters menu item opens [Display parameters](#) dialog box (4.1), which allows you to build the atoms bonds and control the appearance of the OpenGL objects.

Note: This command is not available if there are no atoms.

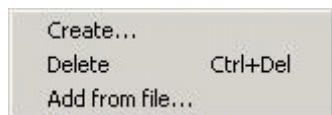
3.2.4.2 Zoom menu item

Use this command to magnify or miniaturize the structure image on your screen. Hold the left mouse button and move mouse in the direction indicated by the mouse pointer to increase or decrease the structure image. Hold the right mouse button to rotate the image. To cancel this command uncheck the Zoom menu item or use the toolbar shortcut. To fit the structure image to the screen press the spacebar.

Note: This command is not available if there are no atoms.

Shortcuts: toolbar: 

3.2.5 Lattice menu



The Lattice menu offers the following menu items:

3.2.5.1 Create menu item

Use this command to display the [Lattice Builder](#) dialog box (4.2), which allows you to build or rebuild the crystal.

Note: This command is not available if the Lattice Builder dialog is opened.

Shortcuts: Toolbar: 

3.2.5.2 Delete menu item

Use this command to delete the current structure.

Note: The command is not available if there is not a structure.

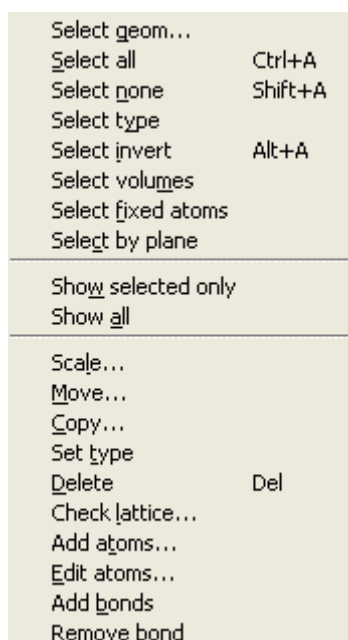
Shortcuts: Keys:Ctrl+Del

3.2.5.3 Add from file menu item

Use this command to display the standard Open dialog box. Use it to locate the *.vnd file on your computer or network from which you wish extract the structure and add to the existing one.

Note: Only the atoms will be added. The unit cell parameters and other data will be not changed.

3.2.6 Operations menu



The Operations menu offers the following menu items:

3.2.6.1 Select geom... menu item

Use this command to open [Select geom...](#) dialog box (4.3), which allows you to select the atoms using the [Box](#) (4.3.1), [Sphere](#) (4.3.2) and [Cylinder](#) (4.3.3) tabs of this dialog box.

3.2.6.2 Select all menu item

Use this command to select all atoms of the structure.


Note: This command is not available if all atoms have already been selected.

Shortcuts: Toolbar: ; keys: CTRL+A

3.2.6.3 Select none menu item

Use this command to deselect all atoms of the structure.

Note: This command is not available if there are no the selected atoms.

Shortcuts: Toolbar: ; keys: SHIFT+A

3.2.6.4 Select type menu item

Use this command to display [Select type](#) dialog box (4.4), which allows you to select the atoms by the atom type.

Note: This command is not available if there are no atoms.

3.2.6.5 Select invert menu item

Use this command to toggle the current selection.

Note: This command is not available if there are no atoms.

Shortcuts: Toolbar: ; keys: ALT+A

3.2.6.6 Select volumes menu item

Use this command to select all volumes, which have been defined using [Set volumes](#) dialog box (4.17).

Note: This command is not available if no volumes are defined.

3.2.6.7 Select fixed atoms menu items

This command allows to select the atoms that were fixed by [Add fixed atoms](#) menu item (3.2.7.10) in the [Task](#) menu (3.2.7). These atoms will be selected by yellow color.

Note: This command is not available if the fixed atoms were not added.

3.2.6.8 Select by plane menu items

Use this command to display [Select by plane](#) dialog box (4.5), allowing to specify a plane that divide the structure into two parts.

3.2.6.9 Show selected only menu item

Use this command to display only the selected atoms and hide all other.

Note: This command is not available if there are not the selected atoms.

3.2.6.10 Show all menu item

Use this command to cancel the [Show selected only](#) (3.2.6.9) command action and display all atoms of the structure.

Note: This command is not available if [Show selected only](#) command has not been executed previously.

3.2.6.11 Scale menu item

Use this command to display [Scale coordinate of atom](#) dialog box (4.6), which allows you to scale the atomic coordinates of the selected atoms.

Note: This command is not available if there are no the selected atoms.

3.2.6.12 Move menu item

Use this command to display [Move atoms](#) dialog box (4.7), which allows you to move the selected atoms to the new positions.

Note: This command is not available if there are no the selected atoms

3.2.6.13 Copy menu item

Use this command to display [Copy atoms](#) dialog box (4.8), which allows you to copy the selected atoms to the new positions.

Note: This command is not available if there are no the selected atoms.

3.2.6.14 Set type menu item

Use this command to display [Set type](#) dialog box (4.9), which allows you to set the new type to the selected atoms.

Note: This command is not available if there are no the selected atoms.

3.2.6.15 Delete menu item

Use this command to delete the currently selected atoms.

This command is not available if there are no the selected atoms.

Shortcuts: keys:Del

3.2.6.16 Check lattice menu item

Use this command to display [Check lattice](#) dialog box (4.10), which allows you to measure the atoms separation, the angles between atoms and the torsion angles.

Note: This command is not available if [Check lattice](#) dialog box is open.

3.2.6.17 Add atom menu item

Use this command to display [Add atom](#) dialog box (4.11), which allows you to add new atom to the structure. Also, you can use [List and edit atoms position](#) dialog box (4.12) to add atoms to the current structure.

Note: This command is not available if [Add atom](#) dialog box or [List and edit atoms position](#) dialog box is open.

3.2.6.18 Edit atoms menu item


Use this command to display [List and edit atoms position](#) dialog box (4.12), which allows you to view and edit the atomic position and types. Also, it allows you to add and remove the atoms.

Note: This command is not available if [List and edit atoms position](#) dialog or [Add atom](#) dialog are open.

3.2.6.19 Add bonds menu item

To add the bond hold the shift key and click the two atoms whose bond you wish to build.


Note: This command is not available if the [Auto rebuild](#) check box of the [Bond](#) tab (4.1.2) of the [Display Parameters](#) dialog box (4.1) is checked.

Shortcuts: toolbar: 

3.2.6.20 Remove bonds menu item

To remove the bond hold the shift key and click the bond, which you wish to remove.

Note: This command is not available if the [Auto rebuild](#) check box of the [Bond](#) tab (4.1.2) in the [Display Parameters](#) dialog box (4.1) is checked.

Shortcuts: toolbar: 

3.2.7 Tasks menu



The Tasks menu offers the following menu items:

3.2.7.1 Wall potential menu item

Use this command to display [Set potential for wall](#) dialog box (4.13), which allows you to specify the potential parameters for the walls used in the MD simulation.

Note: This command is not available while the MD simulation is running.

3.2.7.2 Set potential menu item

Use this command to display [Set potential](#) dialog box (4.14), which allows you to specify the potential and the potential parameters for the interatomic interaction for the MD simulation.

Note: This command is not available while the MD simulation is running or there are no atoms.

3.2.7.3 Ewald sum menu item

Use this command to display [Set Ewald sum parameters](#) dialog box (4.15), which allows you to specify the Ewald sum parameters.

Note: This command is not available while the MD simulation is running or there are no atoms.

3.2.7.4 qEq menu item

Use this command to display [Set qEq parameters](#) dialog box (4.16), which allows you to use the qEq model in the current MD simulation.

Note: This command is not available while the MD simulation is running or there are no atoms.

3.2.7.5 Set volumes menu item

Use this command to display [Set volumes](#) dialog box (4.17), which allows you to select the volumes, where you can calculate the thermodynamic parameters.

Note: This command is not available while the MD simulation is running or there are no atoms.

3.2.7.6 Boundary cond... menu item

Use this command to display [Set boundary condition](#) dialog box (4.18), which allows you to set the boundary condition for the MD simulation.

Note: This command is not available while the MD simulation is running or there are no atoms.

Shortcuts: Toolbar: 

3.2.7.7 [Shock waves](#) menu item

Use this command to open the [Shock waves](#) dialog box (4.19), which allows you to set the direction and value of the velocity of the selected atoms. You will be able also to define the step at which apply this velocity.

Note: This command is not available if the simulation is running or number of atoms is 0.

3.2.7.8 [Run...](#) menu item

Use this command to display [Set parameters for run](#) dialog box (4.20), which allows you to specify the MD simulation parameters such as the time step, the number of the time steps, the output options and start the simulation.

Note: This command is not available while the MD simulation is running or there are no atoms.

Shortcuts: Toolbar: 

3.2.7.9 [Reset](#) menu item

Use this command to delete the current document and open the last saved version of the document. When the MD simulation is running you can use this command to abort simulation or detach the simulation process from the GUI shell. After finishing the MD simulations you must do this command otherwise some commands will be unavailable.

Note: This command is not available if the new document has not been saved yet.

Shortcuts: Toolbar: 

3.2.7.10 [Add fixed atoms](#) menu item

This command allows “to freeze” the group of the selected atoms in the current MD simulation. The coordinates of these atoms will not be changed during the whole simulation. To fix atoms you must select wanted group of atoms and click once on this menu item.

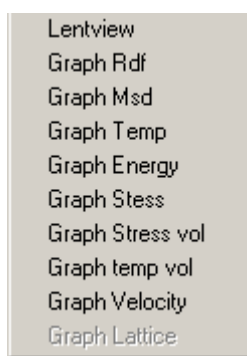
Note: This command is not available if no atoms were selected.

3.2.7.11 [Unfix atoms](#) menu item

This command allows "to unfreeze" all atoms which were fixed by [Add fixed atoms](#) (3.2.7.10) command.

Note: This command is not available if no atoms were fixed.

3.2.8 Results menu



The Results menu offers the following commands:

Lentview	Use this command to display the Lentview program's dialog, which allows you to view the changes of the structure during simulation process. This command is available only after simulation is done.
Graph Rdf	Allows viewing the radial distribution function (RDF) graph, of the selected volume. This graph is not available if before simulation any volume was not selected.
Graph Msd	Allows viewing the mean-square deviation (MSD) function graph, of the selected volume. This graph is not available if before simulation any volume was not selected.
Graph Temp	Allows viewing the Temperature graph.
Graph Energy	Allows viewing the total Energy graph.
Graph Stress	Allows viewing the graphs of the external Pressure and its components Px, Py, Pz. This graph is available if the stress calculation during the MD simulation was turned on [to turn on stress calculation use the Set parameters for run dialog box (4.20)].
Graph Stress vol	Allows viewing the external Pressure and its components graphs of the selected volumes. This graph is available if the stress calculation during the MD simulation was turned on and before MD simulation volume was selected.
Graph Temp vol	Allows to view the temperature graph of the selected volumes, This graph is not available if before simulation any volume was not selected.
Graph Velocity	Allows viewing the Velocity components graphs Vx, Vy, Vz. This graph is not available if before simulation any volume was not selected.
Graph Lattice	This command allows viewing 3D Lattice structure.

The Graphs ... menu items allow you to view all necessary graphs (Temperature, Energy, Pressure, Velocity, MSD and RDF) after the current MD simulation is done. The time step of all graphs depends on value Save step parameter, which may specified in the [Set parameters for run](#) dialog box (4.20). You can easily manipulate with this data, copy to the MS Excel or MS Word, change the axis, line, titles properties and so on.

[Set Graph Title](#) dialog box (4.21)

Allows to change graph and axis titles and fonts. To open this dialog double click on the desired title.

[Axis](#) dialog box (4.22)

Allows to change axis properties. To open this dialog double click on the desired axis.

[Line](#) dialog box (4.23)

Allows to change graph line style. To open this dialog double click on the desired line

To copy the graphs data to the MS Excel activate the graph window and use Ctrl + C keyboard shortcut. Start MS Excel and use Ctrl + V shortcut to paste the graph data on MS Excel sheet. To paste the graph to MS Word use “Paste special” command from the “Edit” menu of this application.

3.2.9 Graph menu



The Graph menu offers the following commands:

Temperature Allows viewing the Temperature graph.

Volumes Temp Allows viewing the temperature graph of the selected volume.

The all aforesaid in the preview section about manipulating with graphical data and setting graph's properties is correctly for this graphs.

3.3 SageMD main window Toolbar



The toolbar is displayed across the top of the application window, below the menu bar. The toolbar provides quick mouse access to many tools used in **SageMD**,

To hide or display the Toolbar, choose Toolbar from the View menu (ALT, V, T).

ClickTo



Open a new document.



Open an existing document. **SageMD** displays the Open dialog box, in which you can locate and open the desired file.



Save the active document or template with its current name. If you have not named the document, **SageMD** displays the Save As dialog box.



Print the active document.



Remove selected data from the document and stores it on the clipboard.



Copy the selection to the clipboard.



Insert the contents of the clipboard into the **SageMD** document.



Reverse the last editing.



Reverse the last undo command action.



Create or rebuild the crystal.



Delete the current document and open the last saved version of the document.



Set the boundary condition for the MD simulation.



Run the MD simulation.



Zoom the lattice image.



Select all atoms.



Deselect all atoms.



Toggle the selection.



Add the bond manually.



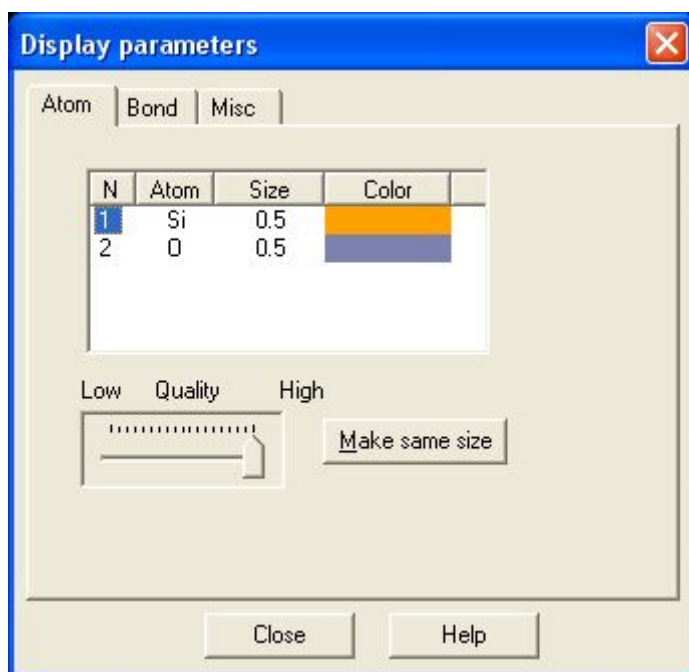
Remove the bond manually.

4 Dialog Boxes

The most of menu items opens the various dialog boxes that allow entering input data and setting essential parameters. The base dialog boxes itemize below in this chapter. All dialog boxes were extracted into the individual chapter for both hyperlinks and text references usability. So, this chapter may be omitted in User Manual reading.

4.1 Display parameters dialog box

Path: [Display](#) menu (3.2.4) → [Parameters](#) menu item (3.2.4.1).



Use this dialog box to build the atomic bonds and to control the atoms size and colors. Also, the dialog allows you to change the appearance the bonds and their radiuses. Using this dialog you can show or hide the bonds and choose the background color. The Display parameters dialog has the following tabs and buttons:

[Atom](#) tab (4.1.1)

[Bond](#) tab (4.1.2)

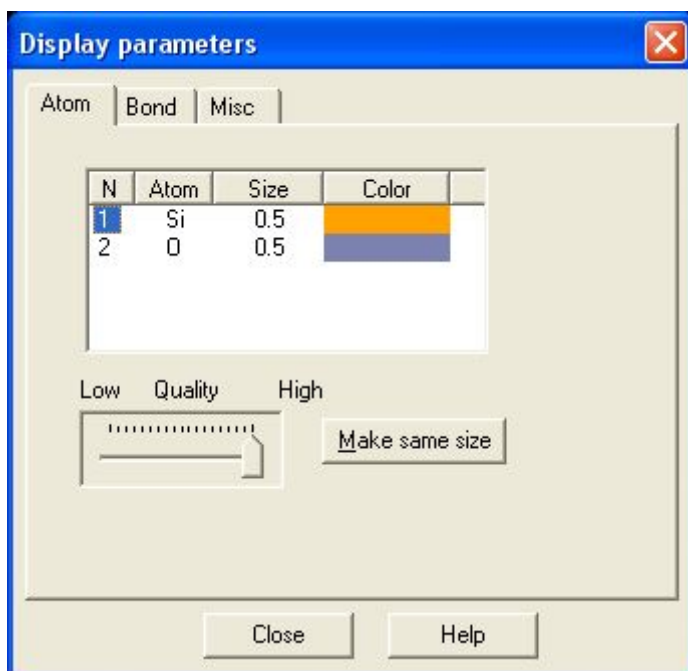
[Misc](#) tab (4.1.3)

Close: use this button to close the dialog.

Help: use this button to get the help about the currently active tab.

4.1.1 Atom tab

Use this tab to change the atomic sizes, colors and the quality of the rendering of the OpenGL graphics.



To change the atoms colors just click on the color you wish to change. The [Color](#) dialog box (4.25) will be displayed. Pick the desired color and click OK button to close the Color dialog.

To change the atoms size click on the value of the atomic radius in the Size column. The dialog will be displayed which allows you to specify the new atomic radius. **Note:** The atomic size is in Angstrom units. The default atomic radius equals its covalent radius.

Use the Quality slider to control the rendering quality of the OpenGL objects. The high value of this parameter in some cases will result to the decreasing of your computer performance. In such case you should decrease the value of this parameter.

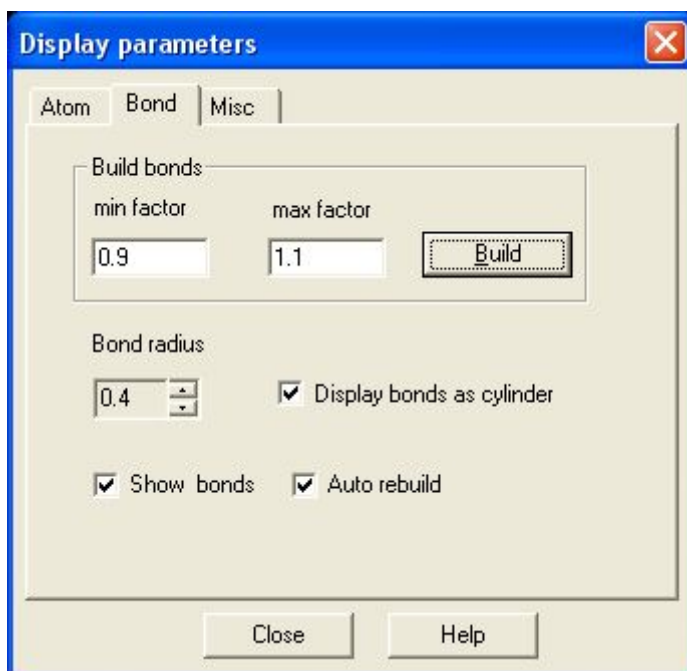
Use Make same size button to make the all atomic radiuses be equal to the radius value of the currently selected atom.

Close: use this button to close the dialog.

Help: use this button to display this page.

4.1.2 Bond tab

Use this tab to build the atoms bonds, change bonds radius, show or hide the bonds image.



This tab has the following boxes and buttons:

Build bonds: group box allows you to create bonds between two atoms if the following criteria is met:

$\text{min factor} * \text{covalent radiuses sum} < \text{distance} < \text{max factor} * \text{covalent radiuses sum}$
where distance = distance between the two atoms forming the bond. To build the bonds click the Build button. If no bonds are shown try another values of the min and max factors.

Display bonds as cylinder: Check this box to display the bonds as a cylinder. Uncheck this box to display the bonds as a cone.

Note: If the atoms forming the bond have the same size the bonds will be displayed as a cylinder in both cases.

Bond radius: Allows you to specify the bond radius as a fraction of the radius of the atoms forming the bond. If these atoms have different radiuses the minimal radius will be used to display the bond thickness. The bond radiuses are in 0-1 range.

Show bonds: Check this box to display the bond images or uncheck to hide it.

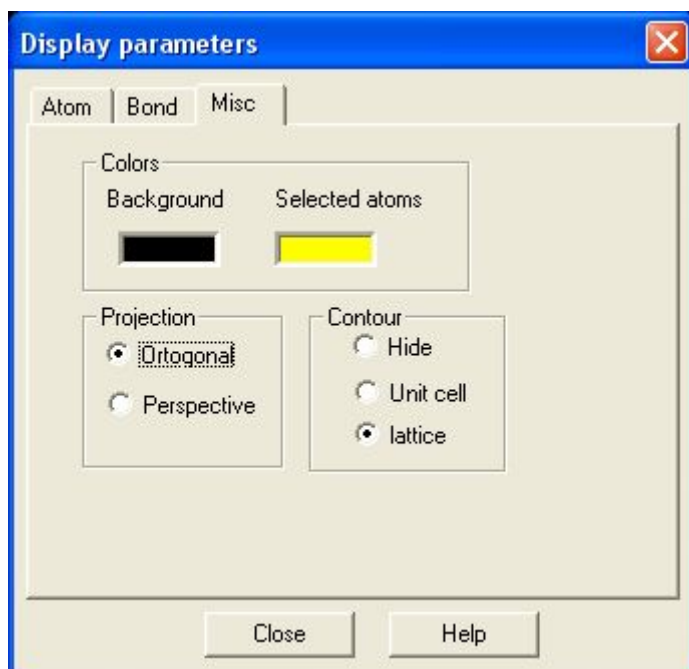
Auto rebuild Uncheck this box to build or remove bonds manually. How to add or remove bonds manually see [Add bonds](#) (3.2.6.19) and [Remove bonds](#) (3.2.6.20) menu items.

Close: use this button to close the dialog.

Help: use this button to display this page.

4.1.3 Misc tab

Use this tab to change various miscellaneous parameters.



This tab has the following boxes and buttons:

Colors: group box allows you to change the window background color and color which is used to display the selected atoms. Just click the appropriate color box to display [Color](#) dialog box (4.25) and choose the new color using this dialog.

Projections: Use this radio button to switch between orthogonal and perspective projections.

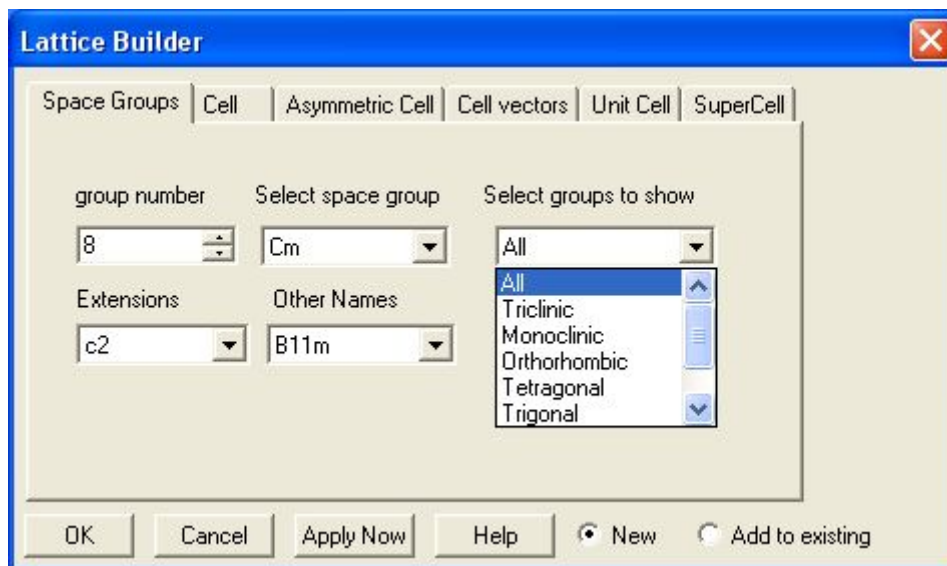
Contour: Allows you to specify how the contour around the crystal will be displayed. Select Hide to hide the contour image. Select Unit cell to display the contour around the unit cell. Select lattice to display the contour around the whole crystal.

Close: use this button to close the dialog box.

Help: use this button to display this page.

4.2 Lattice Builder dialog box

Path: [Lattice](#) menu (3.2.5) → [Create](#) menu item (3.2.5.1).



You can use the Lattice Builder dialog to create new crystal, to modify the space group number, the unit cell parameters, the primitive cell vectors and the box size. Also, using Lattice Builder dialog box you can add, remove atoms from the unit cell or change their types.

The Lattice Builder dialog contains the following tabs and buttons:

[Space Groups](#) tab (4.2.1)

[Cell](#) tab (4.2.2)

[Asymmetric Cell](#) tab (4.2.3)

[Cell vectors](#) tab (4.2.4)

[Unit Cell](#) tab (4.2.5)

[SuperCell](#) tab (4.2.6)

OK: use this button to build or rebuild the crystal using the data from the dialog tabs and to close the dialog.

Cancel: use this button to close the dialog without the building or rebuilding the crystal.

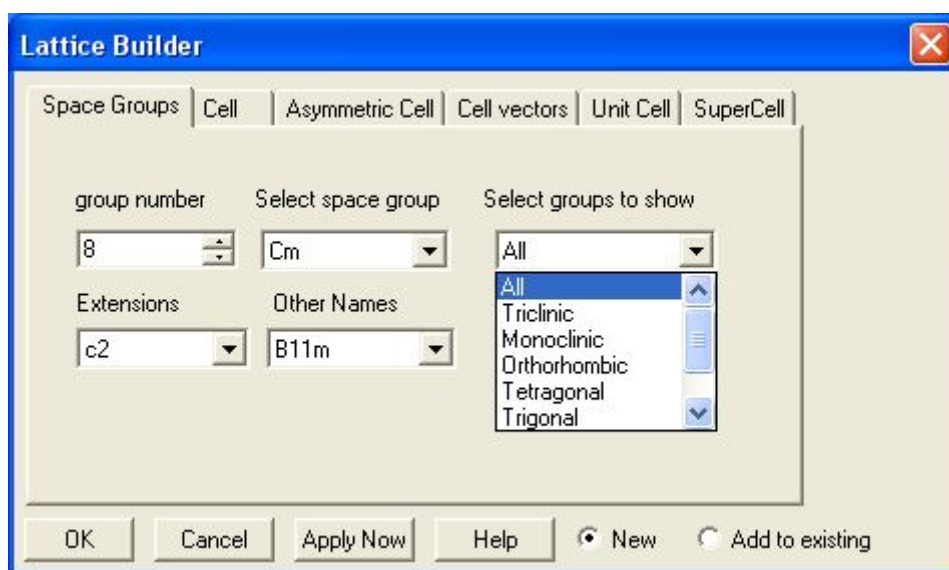
Apply Now: the same as **OK** but the dialog will not be closed.

Help: use this button to get the help about the active tab.

New: if this radio button is checked the current crystal will be deleted before the new crystal will be built.

Add to existing: if this radio button is checked the atoms of the existing structure will not be deleted. New atoms will be added to the existing atoms. However, the existing unit cell settings will be replaced new one.

4.2.1 Space Group tab



The Space Groups tab allows you to specify or modify the space group and space group settings for the structure which you wish to build or rebuild.

The Space Groups tab has the following boxes:

Group number: You can specify a space group number by means of editing this box or using the spin buttons. When you change the group number the contents of the Select space group box will be changed too and vice versa.

Select space group: Enter the space group symbol into this box or select the required space group from the dropdown list. Note: the contents of group number box will be changed to show the number of the selected space group.

Select groups to show: use this box to select the crystal system which space groups you wish to see in the Select space group box. Note that the contents of the group number box will be restricted to show the space groups numbers of the selected crystal system.

Extensions: Allows you to select the space group settings from dropdown list. This box will not be displayed if there is nothing to show.

Other names: Displays the alternate the space group name if any exists. This box will not be displayed if there is not the alternate name for the selected space group.

4.2.2 Cell Tab

The screenshot shows the 'Lattice Builder' dialog box with the 'Cell' tab selected. The 'Cell data' section contains input fields for unit cell parameters. The 'a' field is highlighted with a blue selection box and contains the value '4.91'. The 'b' field contains '4.91' and the 'c' field contains '5.402'. To the right of these fields is the label '(Angstroms)'. Below these are the angle fields: 'alpha' contains '90', 'beta' contains '90', and 'gamma' contains '120'. To the right of these fields is the label '(degrees)'. Below the angle fields, the 'Cristal system' is set to 'Trigonal (Hexagonal axes)'. At the bottom of the dialog are buttons for 'OK', 'Cancel', 'Apply Now', and 'Help', followed by two radio buttons: 'New' (which is selected) and 'Add to existing'.

Parameter	Value	Unit
a	4.91	Angstroms
b	4.91	Angstroms
c	5.402	Angstroms
alpha	90	degrees
beta	90	degrees
gamma	120	degrees

Cristal system: Trigonal (Hexagonal axes)

Buttons: OK, Cancel, Apply Now, Help, ☒ New, ☐ Add to existing

The Cell tab allows you to specify the length and relative orientation of the unit cell vectors in space. The whole crystal can be built by means of the translation of the unit cell along the directions of the unit cell vectors (see [SuperCell](#) tab). The space group symmetry can constrain the lattice parameters to predefined values. In such cases some parameters will not be available to edit.

a, b, c: The length of the unit cell vectors **a**, **b**, **c**.

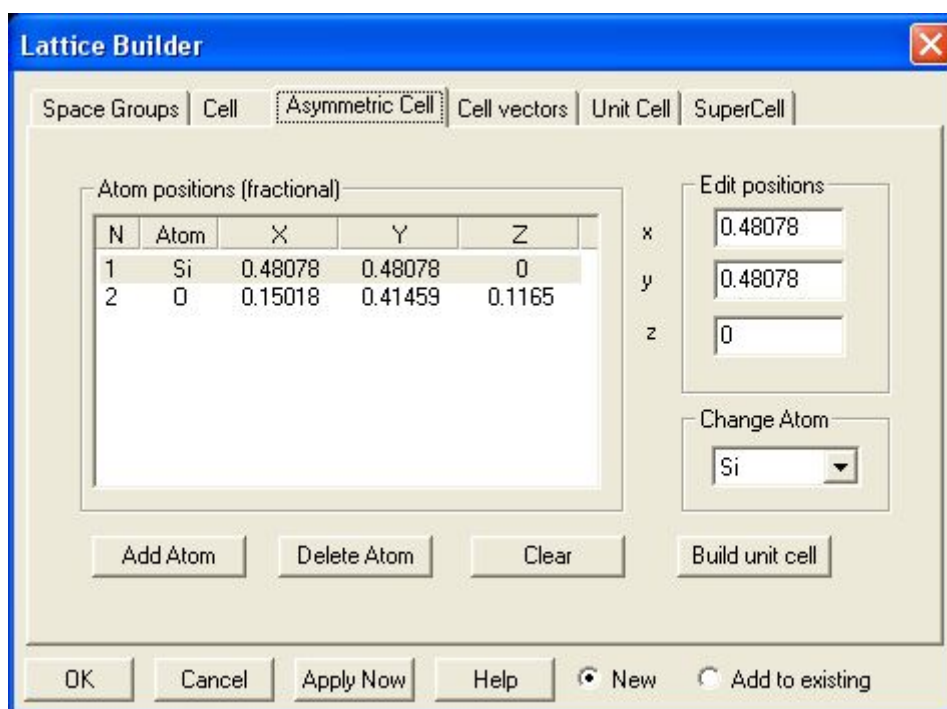
alpha: The angle between b and c vectors.

beta: The angle between a and c vectors.

gamma: The angle between a and b vectors.

Crystal system: Can be one of the seven crystal systems (triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal or cubic. Some of the space groups of the trigonal crystal system can have extensions such as hexagonal or rhombohedral axes.

4.2.3 Asymmetric Cell Tab



Asymmetric Cell tab allows you to build the full unit cell by means of applying the space group symmetry operations for the each atom in the asymmetric cell. It results to the decreasing the amount of the work you need to do for the building of the crystal. Some unit cells contain more then 100 atoms, but asymmetric cell needed to create such unit cell may contain a few atoms only. To build the crystal the **SageMD** uses the data from [Cell](#) (4.2.2), [Unit Cell](#) (4.2.5) and [SuperCell](#) (4.2.6) tabs. The [Space Groups](#) (4.2.1) and this tabs need to build the unit cell only. In fact you can define the position of atoms in the unit cell manually. Then you need to define the cell vectors using the [Cell](#) (4.2.2) tab and specify how many times to repeat the unit cell along cell vectors using the [SuperCell](#) (4.2.6) tab, then press **OK** button to build the crystal.

Asymmetric Cell tab has the following data fields:

Atom positions(fractional): Displays the position and type for the each atom in the asymmetric cell. To edit the atom position or type you can click on the corresponding row in this field.

Edit positions: Allows you to modify the atom positions. x, y and z are the fractional coordinates of the atom. Their values must be a numbers between 0 and 1. If you specify the other value the error message will be displayed.

Change Atom: Allows you to modify the current atom type by selecting the new atom from the dropdown list.

Add Atom: Displays the [Pick element](#) (4.25) dialog which allows you to add the new atom to the asymmetric cell. The default coordinate of the atom are x=0, y=0, z=0. Use the Edit positions boxes to modify these values.

Delete Atom: Click this button to remove an atom from the asymmetric cell

Clear: Click this button to remove all the atoms from the asymmetric cell.

Build unit cell: Click this button to build the full unit cell. The number of atoms and their positions in the unit cell depend on the space group settings [see [Space Group](#) tab (4.2.1)].

4.2.4 Cell vectors tab

The screenshot shows the 'Lattice Builder' dialog box with the 'Cell vectors' tab selected. The tab contains a section titled 'Unit cell vectors (angstroms)' with nine input fields arranged in a 3x3 grid. The values are: Ax = 4.2521847, Ay = -2.4550000, Az = 0.0000000, Bx = 0.0000000, By = 4.9100000, Bz = 0.0000000, Cx = 0.0000000, Cy = 0.0000000, and Cz = 5.4020000. At the bottom, there are buttons for 'OK', 'Cancel', 'Apply Now', and 'Help', along with radio buttons for 'New' (selected) and 'Add to existing'.

Unit cell vectors (angstroms)					
Ax	4.2521847	Ay	-2.4550000	Az	0.0000000
Bx	0.0000000	By	4.9100000	Bz	0.0000000
Cx	0.0000000	Cy	0.0000000	Cz	5.4020000

Use this tab to see the unit cell vectors. The edit boxes of this dialog have the read only permission. To edit the unit cell vectors you can use the [Cell](#) (4.2.2) tab.

ax, ay, az, bx, by, bz, cx, cy, cz: are the Cartesian components of the **a**, **b**, **c** unit cell vectors.

4.2.5 Unit cell tab

The screenshot shows the 'Lattice Builder' dialog box with the 'Unit Cell' tab selected. The tab contains a table of 'Atom positions (fractional)' with columns N, Atom, X, Y, and Z. The table lists 7 atoms: 1 Si (0.48078, 0.48078, 0), 2 Si (0.51922, 0, 0.666667), 3 Si (0, 0.51922, 0.333333), 4 O (0.15018, 0.41459, 0.1165), 5 O (0.58541, 0.73559, 0.783167), 6 O (0.26441, 0.84982, 0.449833), and 7 O (0.73559, 0.58541, 0.216833). To the right of the table is an 'Edit positions' section with input fields for x, y, and z, and a 'Change Atom' dropdown menu set to 'Si'. At the bottom, there are buttons for 'Add Atom', 'Delete Atom', and 'Clear', along with the standard 'OK', 'Cancel', 'Apply Now', and 'Help' buttons, and radio buttons for 'New' (selected) and 'Add to existing'.

N	Atom	X	Y	Z
1	Si	0.48078	0.48078	0
2	Si	0.51922	0	0.666667
3	Si	0	0.51922	0.333333
4	O	0.15018	0.41459	0.1165
5	O	0.58541	0.73559	0.783167
6	O	0.26441	0.84982	0.449833
7	O	0.73559	0.58541	0.216833

Unit Cell tab allows you to view and edit atoms positions in the unit cell. Also, you can change the atom type and add atoms to or remove from the unit cell. Generally, you build the unit cell using the [Asymmetric Cell](#) (4.2.3) tab. Alternatively you can define the atom positions

and their types using this tab. In this case you do not require knowing the space group information and asymmetric cell settings.

The Unit Cell tab has the following data fields:

Atom positions (fractional): Displays the position and type for the each atom in the unit cell. To edit the atom position or type you can click on the corresponding row in this field.

Edit positions: Allows you to modify the atom positions. x, y and z are the fractional coordinates of the atom. Their values must be a numbers between 0 and 1. If you specify the other value the error message will be displayed.

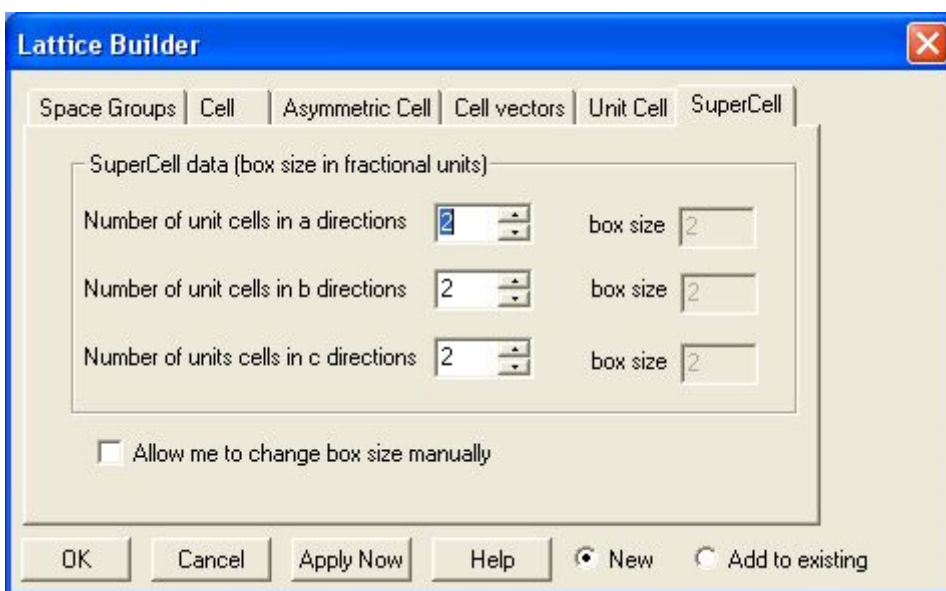
Change Atom: Allows you to modify the current atom type by selecting the new atom from the dropdown list.

Add Atom: Displays the [Pick element](#) (4.25) dialog which allows you to add the new atom to the unit cell. The default coordinate of the atom are $x=0$, $y=0$, $z=0$. Use the Edit positions boxes to modify these values.

Delete Atom: Click this button to remove an atom from the unit cell.

Clear: Click this button to remove all the atoms from the unit cell.

4.2.6 SuperCell tab



The SuperCell tab allows you to create a supercell (crystal) from the current unit cell. Also, you can use this tab to rebuild the supercell. You define the size of the supercell in terms of the numbers of the unit cell in each direction. The fractional coordinates of the supercell are in terms of the unit cell vectors. For example, the fractional coordinates of atoms in 2x2x2 supercell are in 0-1.9999... range. The atoms in the original unit cell have their coordinates in 0-0.9999... range.

The SuperCell tab has the following fields:

Number of unit cell in a direction: Allows you to specify the range of the supercell along the vector of the unit cell.

Number of unit cell in b direction: Allows you to specify the range of the supercell along the b vector of the unit cell.

Number of unit cell in c direction: Allows you to specify the range of the supercell along the c vector of the unit cell.

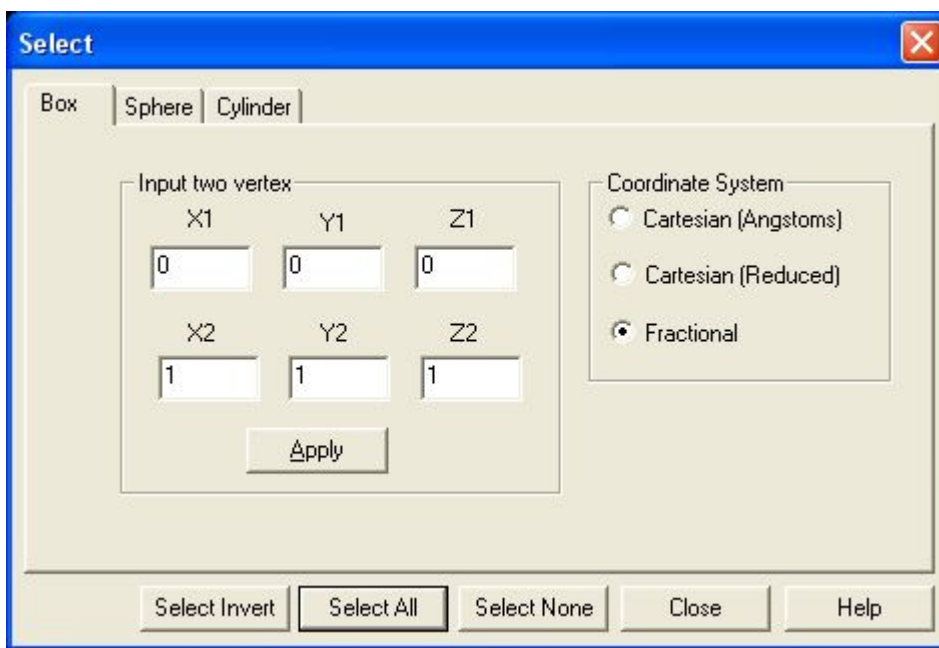
Box size: Defines the periodic box size for MD simulation.

Allow me to change box size manually: By default the box size coincide with the corresponding values in the left box. Check this box to define the box size manually.

4.3 Select geom... dialog box

Path: [Operations](#) menu (3.2.6) → [Select geom...](#) menu item (3.2.6.1).

This dialog allows you to select atoms, which are inside the box, sphere or cylinder.



The [Select geom...](#) dialog contains the following tabs and buttons:

[Box](#) tab (see 4.3.1)

[Sphere](#) tab (see 4.3.2)

[Cylinder](#) tab (see 4.3.3)

Select invert: use this button to toggle the current selection.

Select all: use this button to select all atoms of the structure.

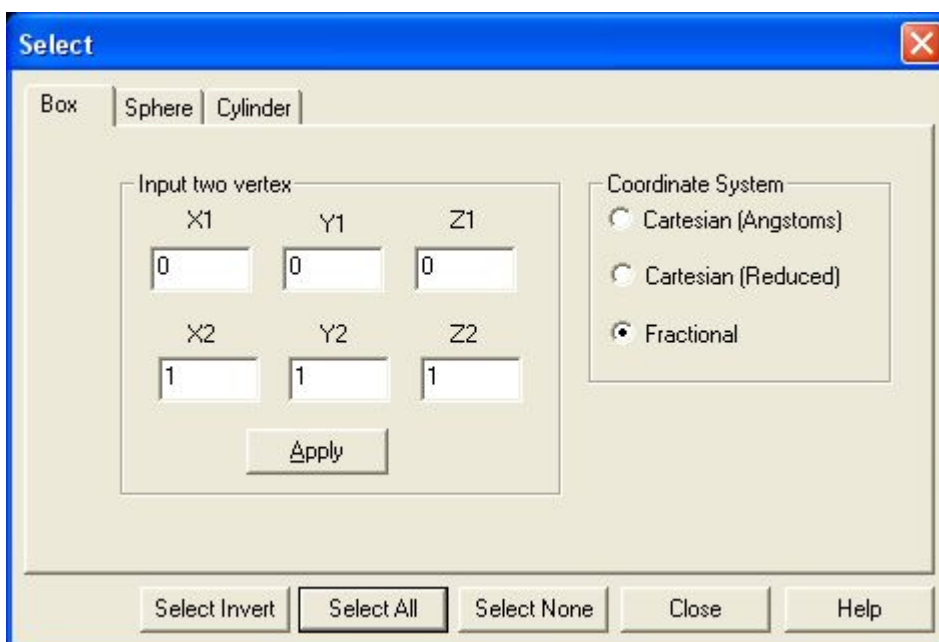
Select none: use this button to deselect all atoms of the structure.

Close: use this button to close this dialog.

Help: use this button to get the help about the currently active tab.

4.3.1 **Box** tab

This tab allows you to specify the box, which contains the atoms you wish to select. To specify the box you need to define the coordinates of the two vertex of this box. These vertexes are the end points of the largest diagonal of the box.



The screenshot shows a software window titled "Select" with a blue title bar and a red close button. Inside, there are three tabs: "Box", "Sphere", and "Cylinder". The "Box" tab is selected. Below the tabs, there is a section labeled "Input two vertex" containing six input fields arranged in two rows. The first row is labeled X1, Y1, Z1 and contains the values 0, 0, 0. The second row is labeled X2, Y2, Z2 and contains the values 1, 1, 1. Below these fields is an "Apply" button. To the right of the input fields is a "Coordinate System" section with three radio buttons: "Cartesian (Angstroms)", "Cartesian (Reduced)", and "Fractional". The "Fractional" option is selected. At the bottom of the window are five buttons: "Select Invert", "Select All", "Select None", "Close", and "Help".

This tab has the following data fields:

X1, Y1, Z1: Allows you to specify the coordinates of the first vertex in the currently active coordinate system.

X2, Y2, Z2: Allows you to specify the coordinates of the second vertex in the currently active coordinate system.

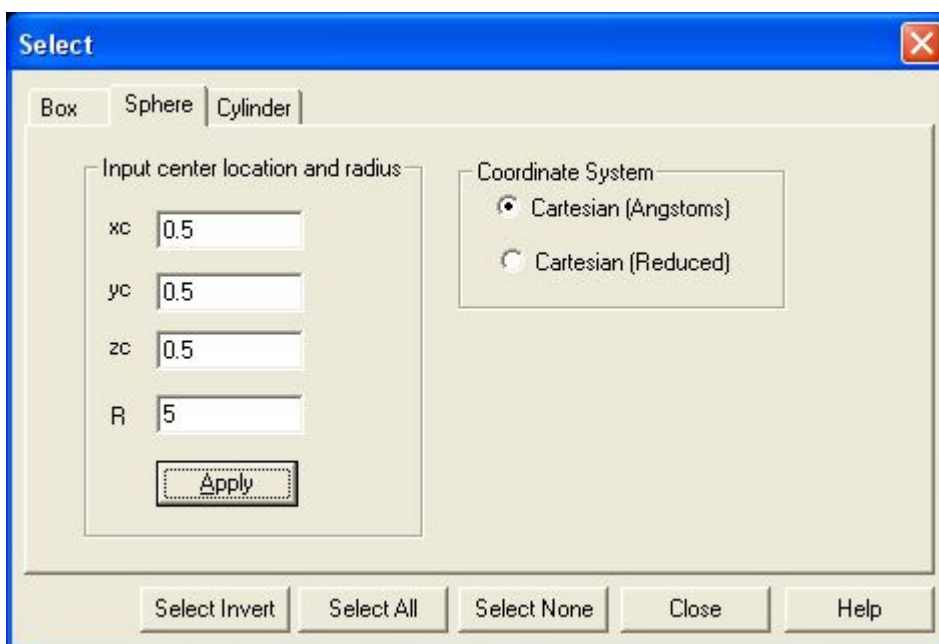
Coordinate system: Allows you to specify which coordinate system to use to define the box.

Note: the reduced factor equals to the length of the **a** vector of the unit cell.

Apply: Click this button to select the atoms, which are inside of the specified box.

4.3.2 Sphere tab

This tab allows you to specify the sphere, which contains the atoms you wish to select. To specify the sphere you need to define the coordinates of the sphere center and the sphere radius.



The image shows a software dialog box titled "Select" with a blue title bar and a red close button. It has three tabs: "Box", "Sphere", and "Cylinder". The "Sphere" tab is selected. Inside the dialog, there are two main sections. The left section, titled "Input center location and radius", contains four input fields: "xc" with the value "0.5", "yc" with "0.5", "zc" with "0.5", and "R" with "5". Below these fields is an "Apply" button. The right section, titled "Coordinate System", contains two radio buttons: "Cartesian (Angstroms)" which is selected, and "Cartesian (Reduced)". At the bottom of the dialog are five buttons: "Select Invert", "Select All", "Select None", "Close", and "Help".

This tab has the following data fields:

xc, yc, zc: Allows you to specify the coordinates of the sphere center.

R: Allows you to specify the sphere radius.

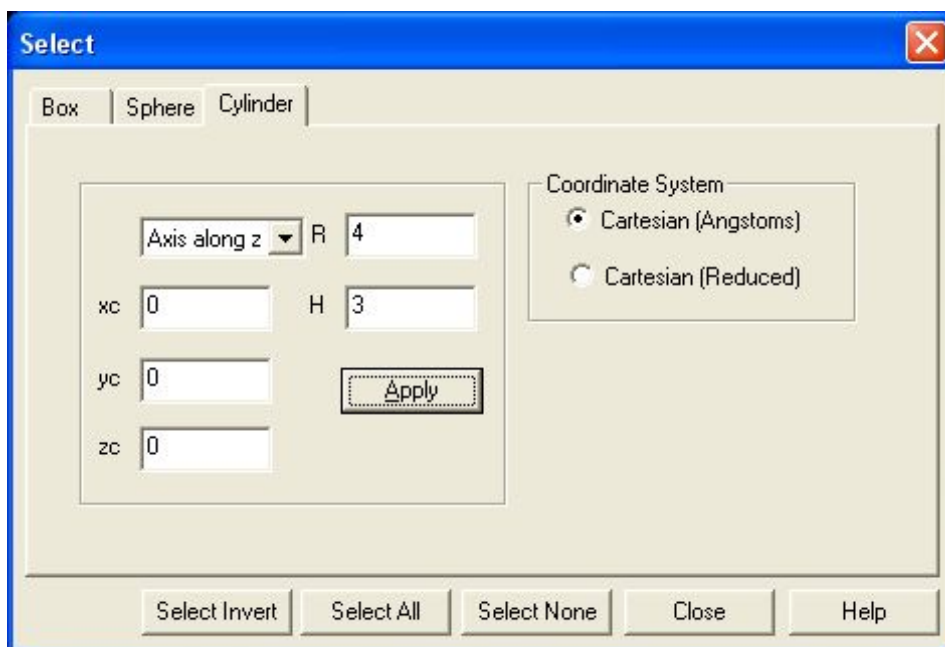
Coordinate system: Allows you to specify which coordinate system to use to define the sphere.

Note: the reduced factor equals to the length of the **a** vector of the unit cell.

Apply: Click this button to select the atoms, which are inside of the specified sphere.

4.3.3 Cylinder tab

This tab allows you to specify the cylinder, which contains the atoms you wish to select. To specify the cylinder you need to define the cylinder axis, the coordinates of the cylinder base center, the cylinder radius and height.



This tab has the following data fields:

Axis along z: Allows you to select from dropdown list the axis along which the cylinder will be orientated.

xc, yc, zc: Allows you to specify the coordinates of the cylinder base center.

R: Allows you to specify the cylinder radius.

H: Allows you to specify the cylinder height.

Coordinate system: Allows you to specify which coordinate system to use to define the sphere.

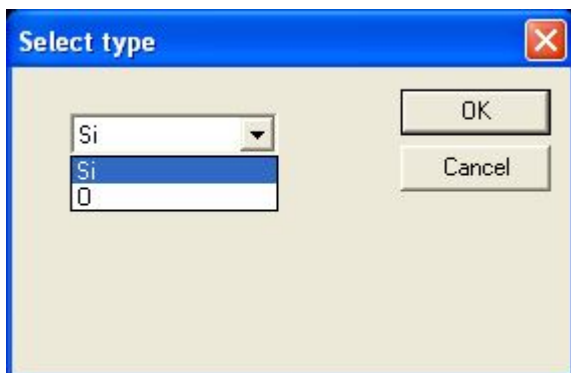
Note: the reduced factor equals to the length of the **a** vector of the unit cell.

Apply: Click this button to select the atoms, which are inside of the specified cylinder.

4.4 Select type dialog box

Path: [Operations](#) menu (3.2.6) → [Select type](#) menu item (3.2.6.4).

Use this dialog to select atoms by the atom type.

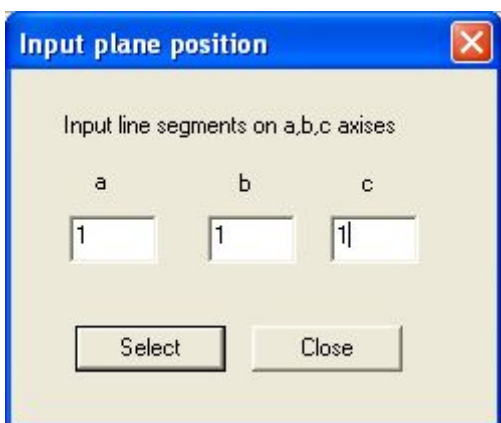


Select the atomic symbol from the dropdown list and click OK button. All atoms, which have the selected type, will be selected.

4.5 Select by plane dialog box

Path: [Operations](#) menu (3.2.6) → [Select by plane](#) menu item (3.2.6.8).

This command of the **SageMD** code allows specifying a plane that divides the structure into two parts. One of these parts will be selected after you click on the Select button of this dialog. Also you can cancel selection by clicking Close button.

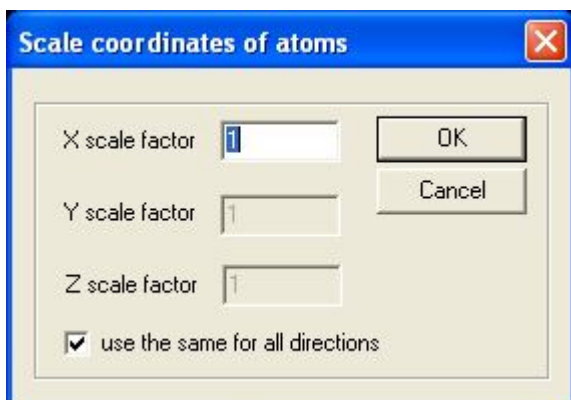


The Select by plane dialog contains three fields **a**, **b** and **c** where you can specify the plane position in fractional coordinate system. After this you can click the Select button, and selected atoms will be displayed in the main window by yellow color. If you want to select another part of the structure just click Invert selection button on the toolbar, or press Alt+A in the keyboard, or choose this command in the Operation menu.

4.6 Scale coordinates of the atoms dialog box

Path: [Operations](#) menu (3.2.6) → [Scale](#) menu item (3.2.6.11).

Use this dialog to scale the coordinates of the selected atoms by the factors you define.



The dialog has the following boxes and buttons:

X scale factor: Allows you to specify the factor to scale X coordinates of the selected atoms.

Y scale factor: Allows you to specify the factor to scale Y coordinates of the selected atoms.

Z scale factor: Allows you to specify the factor to scale Z coordinates of the selected atoms.

use the same for all directions: Check this box to scale all the coordinate components by the same factor.

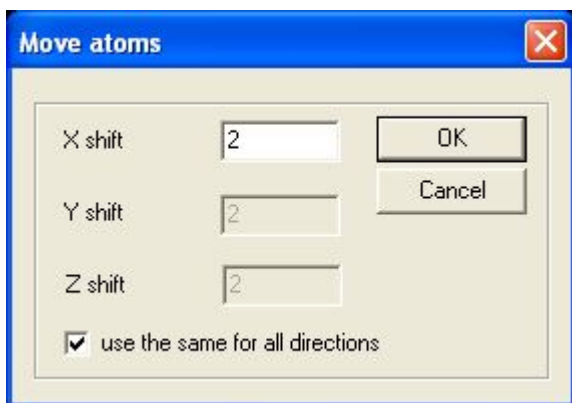
OK: Click this button to scale the atomic coordinates and close the dialog.

Cancel: Click this button to close dialog without the scaling.

4.7 Move atoms dialog box

Path: [Operations](#) menu (3.2.6) → [Move](#) menu item (3.2.6.12).

Use this dialog to move selected atoms by the shift vector you define. All the vector components are in the fractional coordinate system. **x** is directed along the **a**, **y** along the **b**, **z** along **c** vectors of the unit cell.



The dialog has the following boxes and buttons:

X shift: Allows you to specify the shift along a vector of the unit cell.

Y shift: Allows you to specify the shift along b vector of the unit cell.

Z shift: Allows you to specify the shift along c vector of the unit cell.

use the same for all directions: Check this box to move the selected atoms by the same shift in all directions.

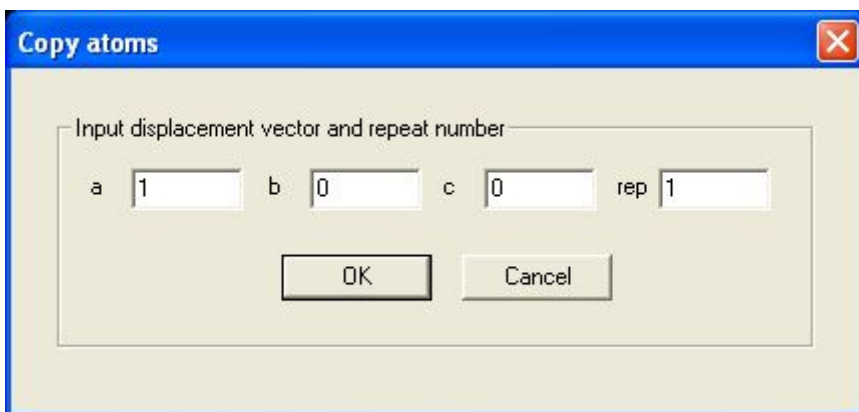
OK: Click this button to move the selected atoms and close the dialog.

Cancel: Click this button to close dialog without the moving.

4.8 Copy atoms dialog box

Path: [Operations](#) menu (3.2.6) → [Copy](#) menu item (3.2.6.13).

This dialog allows you to translate the selected group of atoms in any direction and repeat the displacement one or more times. All the displacement vector components are in the fractional coordinate system. X is directed along a, y along b, z along c vectors of the unit cell.



The dialog has the following boxes and buttons:

a: Allows you to specify the shift along the a vector of the unit cell.

b: Allows you to specify the shift along the b vector of the unit cell.

c: Allows you to specify the shift along the c vector of the unit cell.

rep: Allows you to specify how many times to repeat this operations.

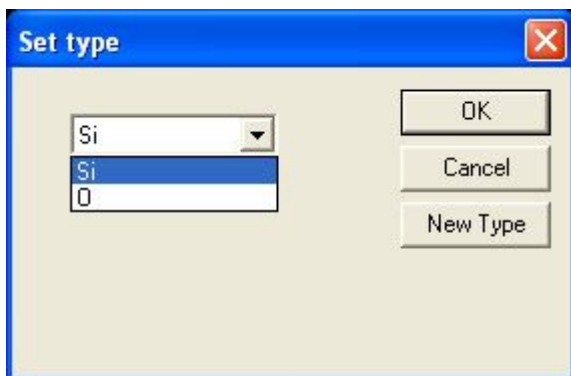
OK: Click this button to copy the selected atoms and close the dialog.

Cancel: Click this button to close dialog without the copying.

4.9 Set type dialog box

Path: [Operations](#) menu (3.2.6) → [Set type](#) menu item (3.2.6.14).

Use this dialog to set the type, which you define to the selected atoms.



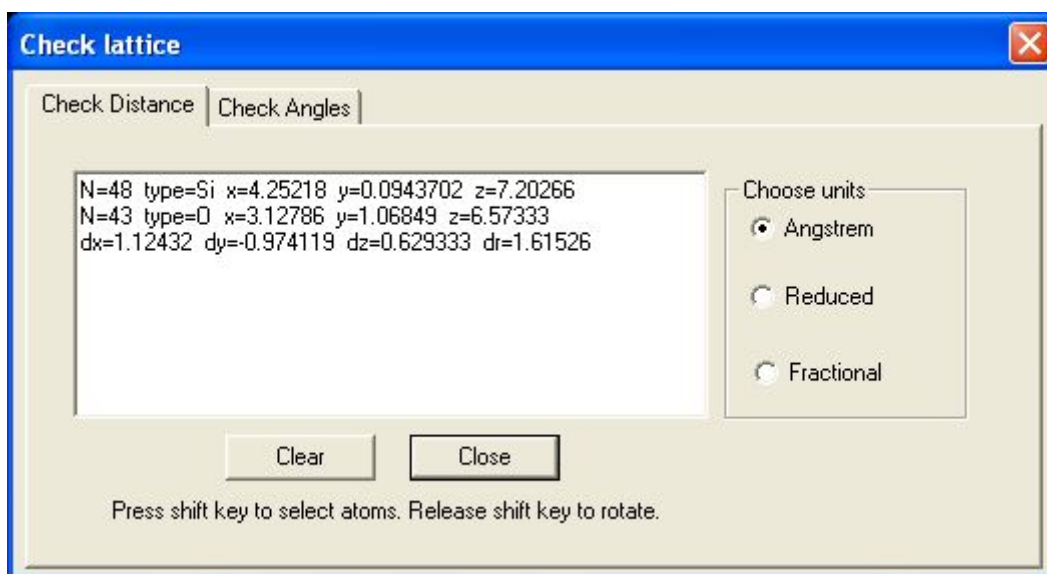
Select the atomic symbol from the dropdown list or click [New Type](#) button to display [Pick element](#) (4.24) dialog, which allows you to pick the new atom type from the table. Then click

OK button to set the new type to the all selected atoms or click Cancel button to close the dialog without the setting new type.

4.10 Check lattice dialog box

Path: [Operations](#) menu (3.2.6) → [Check lattice](#) menu item (3.2.6.16).

The Check lattice dialog box allows to measure atoms separation, angels between atoms and the torsion angels. You can see the positions and atoms separation in fractional, reduced or Cartesian coordinate systems.



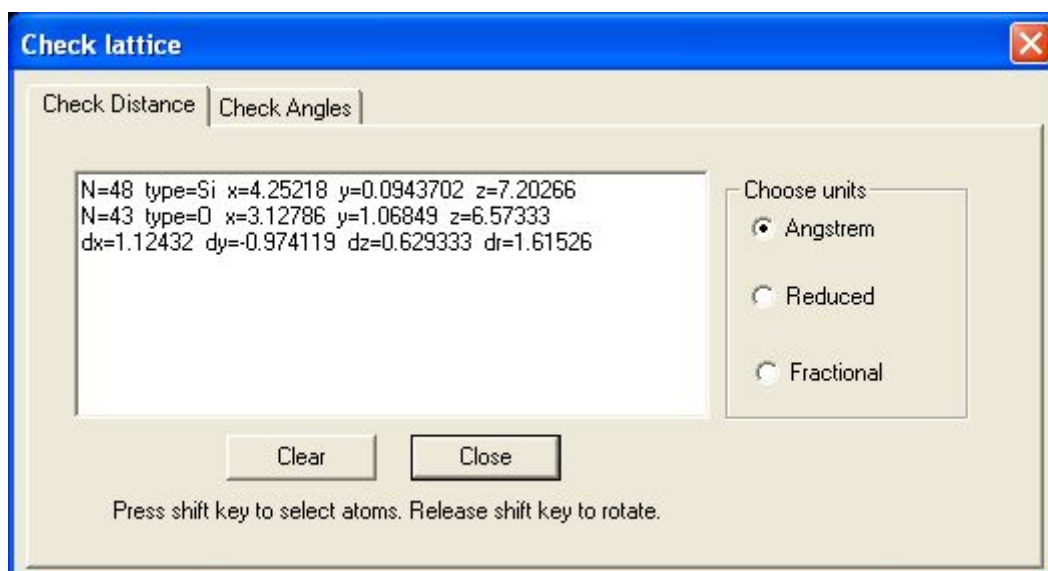
The Check lattice dialog box contains the following tabs:

[Check Distance](#) tab (4.11.1)

[Check Angels](#) tab (4.11.2)

4.10.1 Check distance tab

The Check distance tab allows you to measure the atoms separation. Hold the shift key and click the two atoms whose separation you wish to measure. In the edit box of this tab will be shown up the number of selected atoms, its types and positions. In the third line will be appeared the atoms separation.



The Check distance tab contains the following fields and buttons:

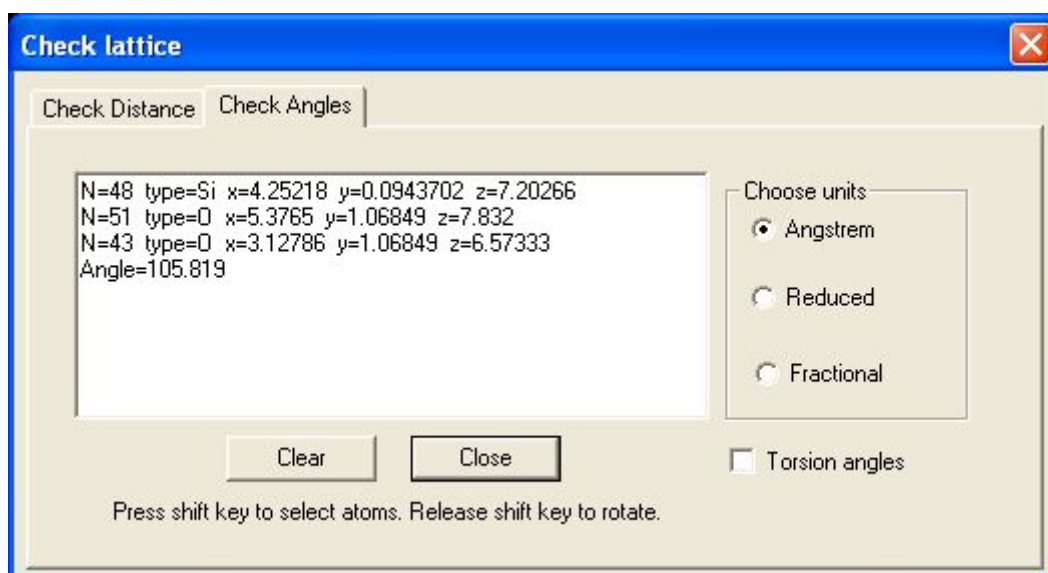
Chose units: allow you to choose the coordinate system in which the atoms separation and positions will be shown.

Clear: use this button to clear the edit box of this tab.

Close: use this button to close this dialog.

4.10.2 Check angles tab

The Check Angles tab allows you to measure the angles between atoms and the torsion angles. Hold the shift key and click the three atoms to measure the angle between them. At first you need to click the atom, which is the vertex of the angle. To measure the torsion angle you must check the Torsion angles radio button. Then hold the shift key and click the two atoms B and C whose angle you wish to measure. Then click the two atoms A and D, which are bonded to B and C respectively. In the edit box of this tab will be shown up the number of selected atoms, its types and positions. In the last line will be appeared the angle between atoms or torsion angle.



The Check Angles tab contains the following fields and buttons:

Chose units: allows choosing the coordinate system in which the atoms separation and positions will be shown.

Clear: use this button to clear the edit box of this tab.

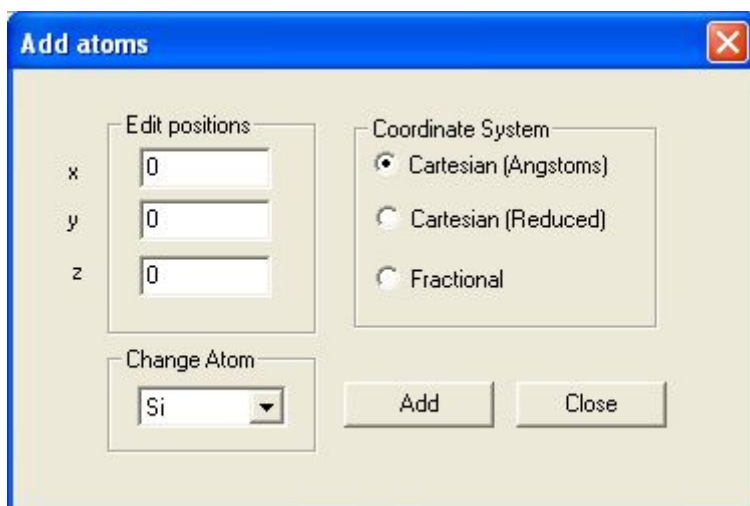
Close: use this button to close this dialog.

Torsion angels: use this check box to measure the torsion angles.

4.11 Add atoms dialog box

Path: [Operations](#) menu (3.2.6) → [Add atoms](#) menu item (3.2.6.17).

The Add atom dialog allows you to add new atom to the structure. You can specify the atomic positions and type.



The Add atoms dialog contains the following fields and buttons:

Edit positions: Allows you to modify the atom positions.

Coordinate system: Use this field to choose the coordinate system. You can choose Cartesian, reduced or fractional coordinate system.

Note: the reduced factor equals to the length of a vector of the unit cell.

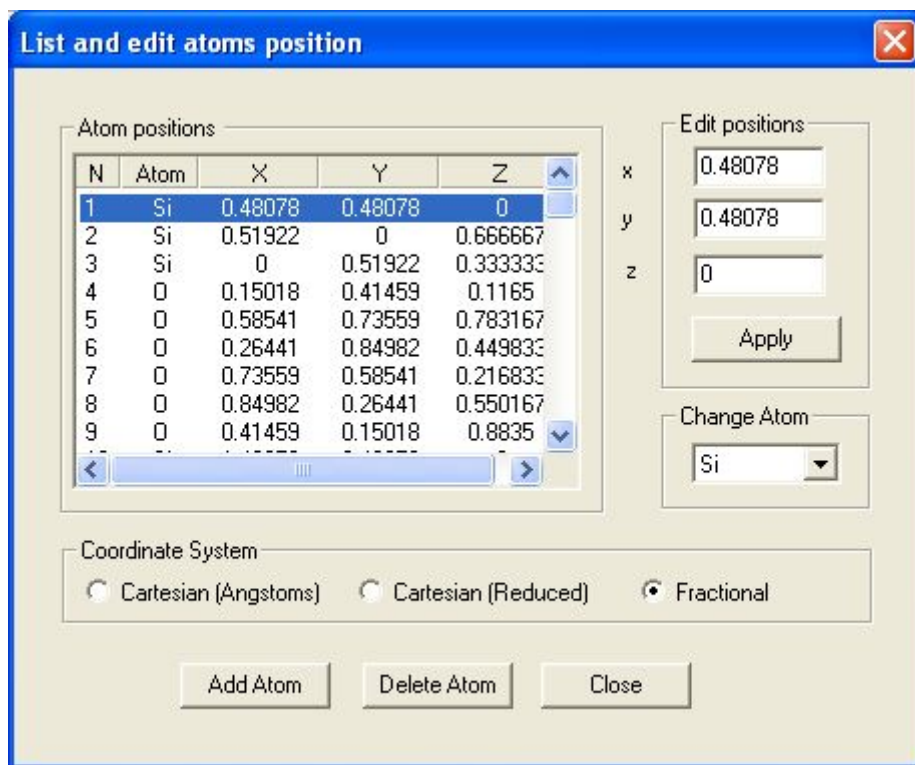
Change Atom: Allows you to modify the current atom type by selecting the new atom from the dropdown list.

Add: Use this button to add the new atom to the structure.

Close: Click this button to close this dialog.

4.12 List and edit atoms position dialog box

Path: [Operations](#) menu (3.2.6) → [Edit atoms](#) menu item(3.2.6.16).



This dialog allows you to view and edit the atomic position and types. Also, it allows you to add and remove the atoms. Using this dialog you can see and edit the position of individual atom in the opened document. Just click on the atom in the structure image and you can see the selected line with atomic position in the Atom positions field. You can edit the coordinates of the selected atom using the Edit positions boxes and change the atom type using Change atom dropdown list. Also you can select the individual atom in the Atom positions field and it will be selected in the structure image.

The List and edit atoms position dialog contains the following fields and buttons:

Atom positions: Displays the position and type for the each atom of the current structure. To see the location of the atom in structure image or to edit the atom position and type you can click on the corresponding row in this field.

Edit positions: Allows you to modify the atom positions.

Note: you need to click Apply button to apply your edit action.

Apply: Use this button to change the atom position accordingly to the values in the Edit positions boxes.

Change atom: Allows you to modify the current atom type by selecting the new atom from the dropdown list.

Coordinate system: Use this field to choose the coordinate system. You can choose Cartesian, reduced or fractional coordinate system.

Add Atom: Use this button to add the new atom to the structure. Atom type is specified in the Change atom box. The default coordinate of the atom are $x=0$, $y=0$, $z=0$. Use the Edit positions boxes to modify these values.

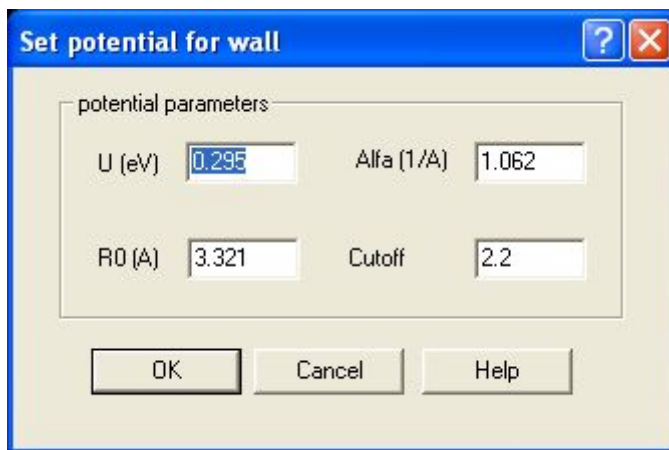
Delete Atom: Click this button to remove an atom from the unit cell.

Close: Click this button to close this dialog.

4.13 Set potential for wall dialog box

Path: [Tasks](#) menu (3.2.7) → [Wall potential](#) menu item (3.2.7.1).

The Set potential for wall dialog allow you to specify the parameters of the Morse potential $U(r)=u*[exp(-2*Alfa*(r-R0))-2*exp(-Alfa*(r-R0))]$ on the box walls.



The Set potential for wall dialog contains the following fields and buttons:

U: Allows you to specify the deep of the potential pit.

Alfa: Allows you to specify the hardness parameter of the Morse potential.

R0: The distance r to the point where the potential has the minimum value ($U(r)=-u$).

Cutoff: Allows you to specify the cutoff radius as the fraction of the $R0$. The real cutoff radius (Angstrom) is $cutoff*R0$.

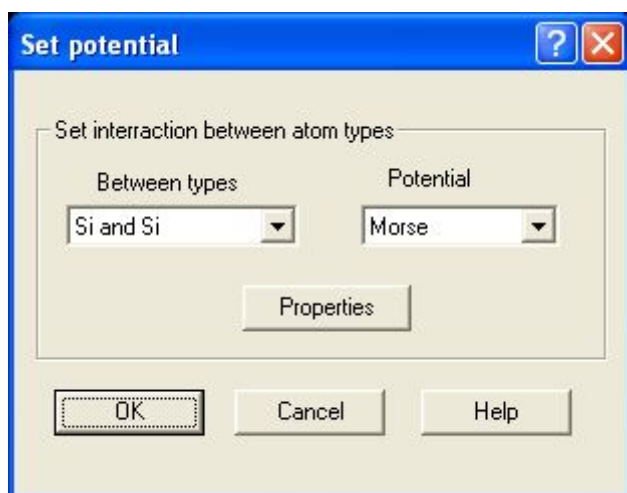
OK: Click this button to set potential parameters for wall and close the dialog.

Cancel: Click this button to close the dialog without saving the wall potential parameters.

4.14 Set potential dialog box

Path: [Tasks](#) menu (3.2.7) → [Set potential](#) menu item (3.2.7.2).

The Set potential dialog allows you to specify the potentials of the interatomic interactions.



The Set potential dialog contains the following fields and buttons:

Between types: Allows you to choose two atoms types between which you want to specify the interatomic potential.

Potential: From the dropdown list select the interatomic potential, which you wish to set for the pair, you selected in Between types box. For many body potentials or if you use the Ewald sum you must set the same potential for all interatomic interactions. The available potentials are EAM, Morse, modified Morse, Bukingem, Watanabe, SW, Tersoff B, Tersoff C, BKS, Abinit, Gaussian98. To use the Abinit and Gaussian98 potentials you need to install these codes on your computer. During the MD simulations the **SageMD** call those codes to calculate the forces. Any pair potential you can represent as EAM potential file, which has only the pair part of the interatomic interaction. The "dens" and "embed" parts of the file you must exclude. Thus, you have the ability to implement the pair potentials, which are not implemented in **SageMD** code. See [EAM potential file format](#) (2.3.3).

Properties: Click this button to display the [Set potential parameters](#) dialog box (4.14.1), which allows specifying the potential parameters of the interatomic interactions. This button is visible not for all interatomic potentials.

Poten file: This button is available only for EAM potential. It allows choosing the potential data file.

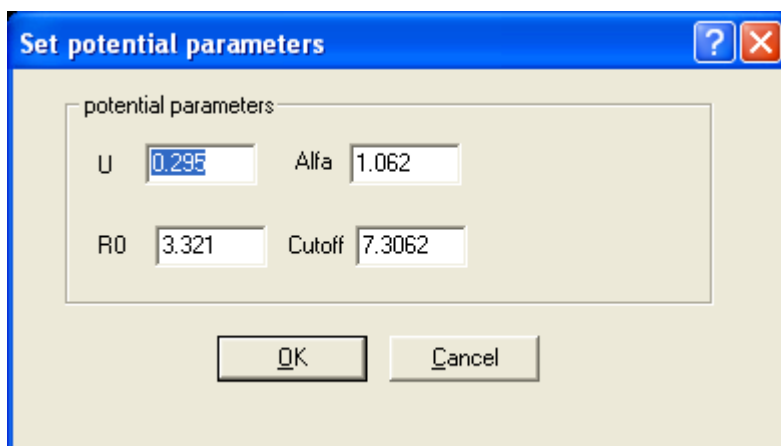
OK: Click this button to set potential and close the dialog.

Cancel: Click this button to close the dialog.

4.14.1 Set potential parameters dialog box

Path: [Tasks](#) menu (3.2.7) → [Set potential](#) menu item (3.2.7.2) → [Set potential](#) dialog box (4.14)

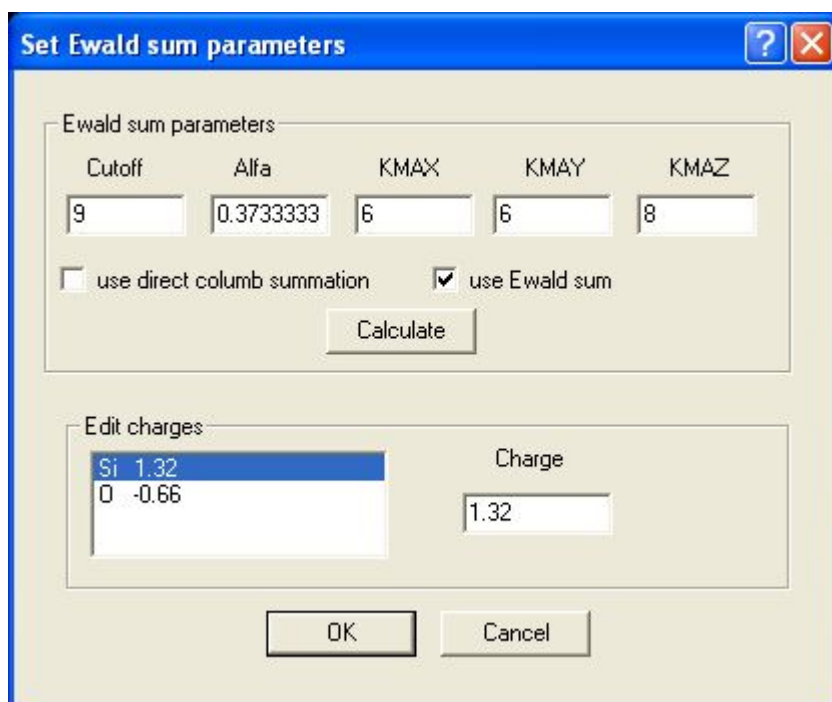
The Set potential parameters dialog box allows you to specify selected potential parameters. The next figure represents Set potential parameters dialog box for Morse potential.



4.15 Set Ewald sum parameters dialog box

Path: [Tasks](#) menu (3.2.7) → [Ewald sum](#) menu item (3.2.7.3).

The Set Ewald sum parameters dialog box allows you to specify long-range electrostatic potentials methods and to set some parameters.



The Set Ewald sum parameters dialog contains the following fields:

Use Ewald sum: Check this box to use Ewald summation in the current simulation. The Ewald summation is the technique for calculating electrostatic interactions in a periodic (or pseudo-periodic) system.

Use direct coulomb summation: Check this box to use direct Coulomb sum in the current simulation. Use of the direct Coulomb sum is sometimes necessary for accurate simulation of isolated (nonperiodic) systems. It is not for periodic systems.

Calculate: Click this button to use automatic calculation of Alfa, KMAX, KMAY, KMAZ parameters. You can enter only Cutoff parameter to use automatic calculation or you can manually specify Alfa, KMAX, KMAY, KMAZ. This button is visible only if use Ewald sum box was checked.

Edit Charges field: Allows you to choose the atom type and specify its charges.

Cutoff: Allows you to specify the real space cutoff forces Radius of long-range correction.

Alfa: Allows you to specify the Ewald convergence parameter Alfa.

KMAX, KMAY, KMAZ: Allows you to specify the Ewald sum parameters that effectively define the range of the reciprocal space sum (one for each of the three axis directions).

There are three variables that control the accuracy the Ewald summation, they are - Alfa the Ewald convergence parameter, Cutoff the real space forces cutoff and the KMAX,Y,Z integers that effectively define the range of the reciprocal space sum (one integer for each of the three axis directions). These variables are not independent and it is usual to regard one of them as pre-determined and adjust the other two accordingly. The Ewald sum splits the (electrostatic) sum for the infinite, periodic system into a damped real space sum and a reciprocal space sum. The rate of convergence of both sums is governed by Alfa. Evaluation of the real space sum is truncated at $r = \text{Cutoff}$ so it is important that Alfa be chosen so that contributions to the real space sum are negligible for terms with $r > \text{Cutoff}$. The recommended value for Alfa is $3.2/\text{Cutoff}$ or greater (too large a value will make the reciprocal space sum very slowly convergent). The optimum values for KMAX are the smallest values that reproduce the correct Coulombic energy and virial at the value of Alfa to be used in the simulation. Note that one needs to specify the three integers (KMAX, KMAY, KMAZ) referring to the three spatial directions, to ensure the reciprocal space sum is equally accurate in all directions. The values of (KMAX, KMAY, KMAZ) must be commensurate with the cell geometry to ensure the same minimum wavelength is used in all directions. For a cubic cell set $KMAX = KMAY = KMAZ$. However, for example, in a cell with dimensions $2A = 2B = C$ (i.e. a tetragonal cell, longer in the c direction than the a and b directions) use $2KMAX = 2KMAY = KMAZ$. If the values for the KMAX used are too small, the Ewald sum will produce spurious results. If values that are too large are used, the results will be correct but the calculation will consume unnecessary amounts of cpu time. The amount of cpu time increases with $KMAX * KMAY * KMAZ$.

4.16 Set QEq parameters dialog box

Path: [Tasks](#) menu (3.2.7) → [qEq](#) menu item (3.2.7.4).

Use this dialog box to turn on the QEq method for the MD simulation. Rappe and Goddard III suggested the charge equilibration (QEq) model to predict the atoms charge distribution in dependence of the molecular geometry.



The dialog has the following fields and buttons:

Use qEq: check this box to use the qEq method during the MD simulation.

Call qeq every N step: means that every N step the atomic charges will be recalculated.

OK: click this button to apply current settings and close dialog.

Cancel: Click this button to discard all changes and close dialog.

The parameters of the QEq model are in the QEq_params.dat file. The example of such file is following below.

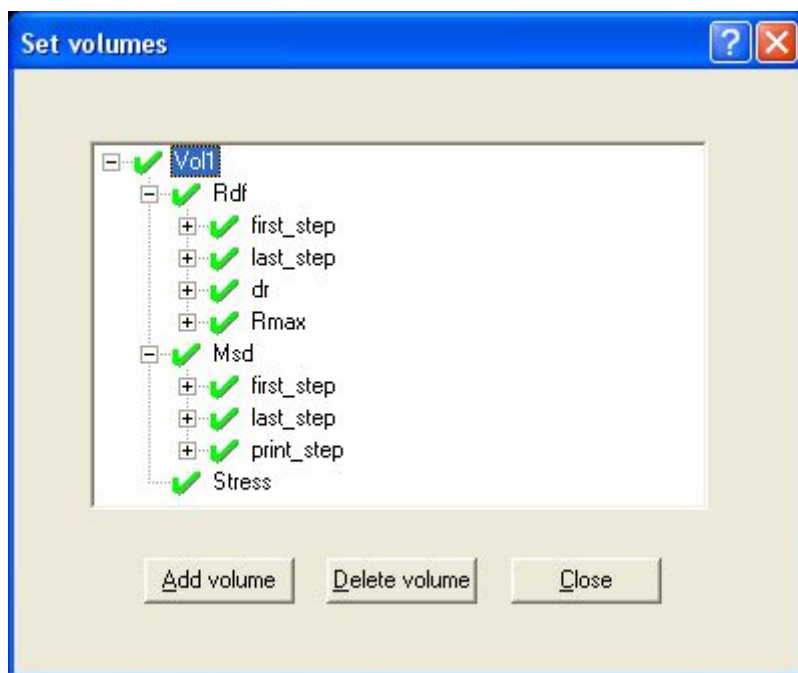
```
#*****
#El    QuanNo MinQ MaxQ  ElectNeg  Hardness  GenRadii
H      1  -1   1  4.52800  6.49205  0.37100
Li     2  -1   1  3.00600  2.38600  1.55700
C      2  -4   4  5.34300  5.06300  0.75900
N      2  -3   5  6.89900  5.88000  0.71500
O      2  -2   6  8.74100  6.68200  0.66900
F      2  -1   7 10.87400  7.47400  0.70600
Na     3  -1   1  2.84300  2.29600  2.08500
Mg     3  -1   2  3.95100  3.69300  1.50000
Al     3  -5   3  4.06000  3.59000  1.20100
Si     3  -4   4  4.16800  3.48700  1.17600
P      3  -3   5  5.46300  4.00000  1.10200
S      3  -2   6  6.92800  4.48600  1.04700
Cl     3  -1   7  8.56400  4.94600  0.99400
K      4  -1   1  2.42100  1.92000  2.58600
Br     4  -1   7  7.79000  4.42500  1.14100
Ti     4  -1   4  3.47000  3.38000  1.60700
Zr     5  -1   4  3.40000  3.55000  1.75800
```

To learn more see original paper²⁶

4.17 Set Volumes dialog box

Path: [Tasks](#) menu (3.2.7) → [Set volumes](#) menu item (3.2.7.5).

Set Volumes dialog box allows to select any atoms in the current structure into independent group, which called volume. These volumes are useful if you want to get some parameters not of the whole structure, but only of the some part of it. You can add up to 20 volumes. To add new volume you must select atoms (see the FAQs Q1) and click Add volume button.



The Set volumes dialog contains the following buttons:

Add volume: Allows to add selected group to the new volume.

Delete volume: Allows to delete selected volumes from the volumes list.

Close: Click this button to close Set volumes dialog.

Set volumes dialog realized in tree-type structure. In the root we can see the selected volumes. The second branches (rdf, msd and stress) contain the parameters to the calculation of the radial distribution function, mean square deviation and stress. To open the second branches click once on the cross.

RDF - Radial Distribution Function. Radial distribution function is a statistical function about the atomic distribution around an atom in a structure. This function describes fluctuations in density around given atom. You can think of it as the average number of atoms found at given distance in all directions.

The RDF branch contains following parameters:

first_step: Allows to specify the initial time step of RDF calculation.

last_step: Allows to specify the final time step of RDF calculation.

dr: Allows to specify the radial step width of RDF.

Rmax: Allows to specify the maximum value of the RDF radius.

MSD - Mean Square Deviation. The mean square displacement contains information on the atomic diffusivity

The MSD branch contains following parameters:

first_step: Allows to specify the initial time step of MSD calculation.

last_step: Allows to specify the final time step of MSD calculation.

print_step: Allows to specify the frequency for saving MSD in the trajectory file.

Stress: Not realized yet.

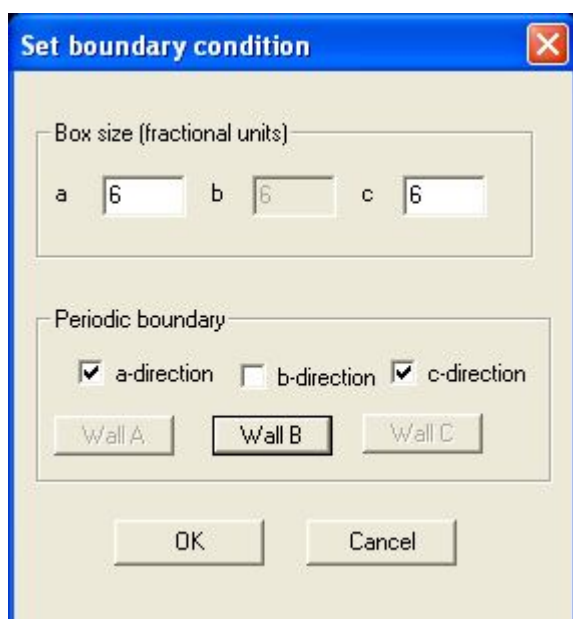
To change or specify any parameter in the RDE, MSD or Stress branches just click once on the required field and enter your value.

Select and click once on the volume name to rename it (the default name is "NoName"). To exclude the volume from the current simulation process just double click on the volume's cross or name (near the name will be appeared red cross instead of green tick).

4.18 Set boundary conditions dialog box

Path: Tasks menu (3.2.7) → Boundary cond... menu item (3.2.7.6).

The Set boundary conditions dialog box allows you to set the boundary conditions for the MD simulation. By default periodic boundary conditions are in effect - this can be altered with this dialog. The periodic boundary conditions can be turned off in any direction independently of the others. When the periodic boundary conditions are turned off in some direction you need to adjust the position and velocity of the potential wall using the Wall button for this direction. Thus, you can simulate free surfaces by setting the wall position beyond the wall potential cutoff distance from the crystal free surface. Also, you can simulate the processes of compression or tension of the crystal by setting none zero wall velocities.



The dialog has the following fields and buttons:

Box size: Allows you to change the size of the simulation box. This option is not available if periodic boundary condition is not set.

Periodic boundary: Allows you to set or unset periodic boundary conditions in a, b and c directions of the unit cell. If in some direction the periodic boundary is turned off you can use the button below to display Moving wall dialog box (4.18.1), which allows you to set the potential wall position and velocity.

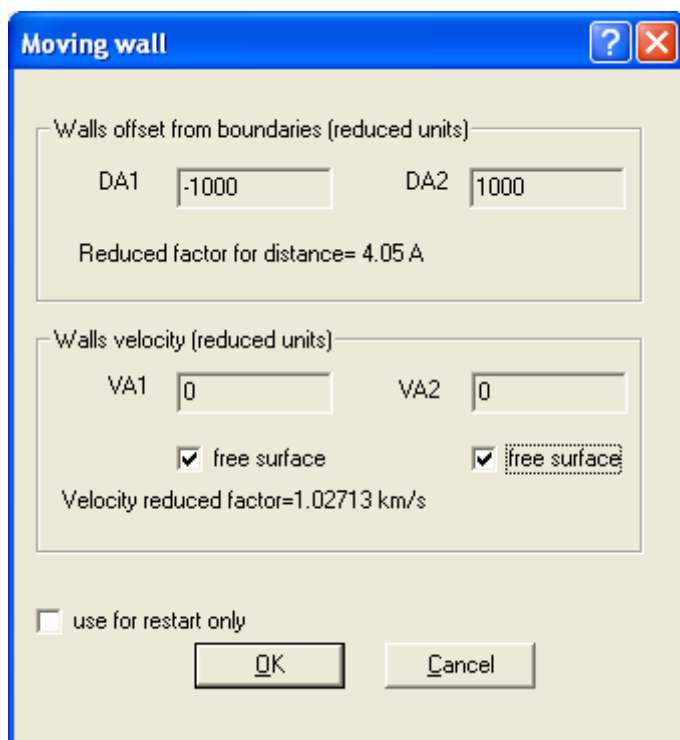
OK: Use this button to apply your changes and close the dialog.

Cancel: Use this button to discard your changes and close the dialog.

4.18.1 Moving wall dialog box

Path: [Tasks](#) menu (3.2.7) → [Boundary cond...](#) menu item (3.2.7.6) → [Set boundary conditions](#) (4.18) dialog box.

The Moving wall dialog box allows you to set the potential wall at specified distance from crystal surface.



The dialog has the following fields and buttons:

Walls offset from boundaries: Allows you to specify distance between the crystal edge and the potential wall in reduced units. Use the left box to specify the distance from the edge, which is the near coordinate system origin. Use the right box to specify parameters for the opposite edge of the crystal. The negative values mean that the potential wall was moved in the negative direction of the coordinate axe from the crystal edge. You specify offset in the reduced units.

Walls velocity: Allows you to specify the value and direction of the wall velocity. Use this feature to model the crystal tension or compression.

Free surface: Check the box or boxes to model the free surface or surfaces of the crystal.

Use for restart only: Check this box to set wall positions and velocities between restarts of the MD simulation. By default, the wall positions and velocities between restarts keep values from previous MD simulation.

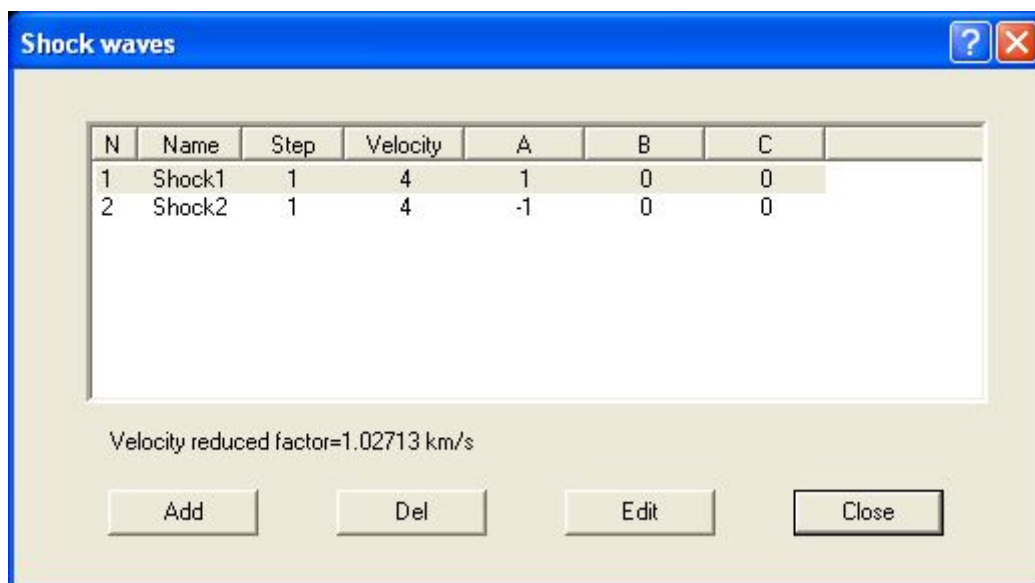
OK: Use this button to apply your changes and close the dialog.

Cancel: Use this button to discard your changes and close the dialog

4.19 Shock waves dialog box

Path: [Tasks](#) menu (3.2.7) → [Shock waves](#) menu item (3.2.7.7).

Use this dialog box to simulate the propagation of the shock waves in the structure or when you need abruptly to set the new value and direction of the selected atoms velocity (the bombarding processes). The initial velocity value is applied at the beginning the step you specify using this dialog. To add shock wave you must select atoms before clicking on the Add button.



The dialog has the following fields and buttons:

N: The number of the shock wave. You have not the possibility to edit this field.

Name: The name of the shock wave. You can leave the default name or type the new one. This field must not be empty.

Step: The step number at which apply the specified initial velocity to the atoms, which were selected for the shock wave. Which atoms were selected you can see by clicking on the desired line. The atoms of the selected wave will be highlighted.

Velocity: the value of the atoms velocity of the shockwave. This value applied as the initial velocity of the shock wave atoms at the beginning of the specified step. You set velocity using the reduced units. The real value (km/s) = Velocity*velocity reduced factor.

A, B, C: define the vector in fractional units along which the velocity vector of the shock wave atoms will be directed. At the example the one shock wave is directed in positive direction of the A vector of the simulation box and another in the negative direction of this vector. The value of the vector is no matter. The direction means only. The (1,1,1) and (5,5,5) vectors have the same direction. So you can specify any of them.

Add: use this button to specify new shock wave from the currently selected atoms.

Del: use this button to delete the currently selected shock wave.

Edit: use this button to change the shock wave parameters. Also, you can double click on the line you wish to edit.

Close: use this button to close the dialog.

4.20 Set parameters for run dialog box

Path: [Tasks](#) menu (3.2.7) → [Run...](#) menu item (3.2.7.8).

The Set parameters for run dialog box allow you to specify the MD simulation parameters.

Set parameters for run

General options

Time step: 0.01

Number steps: 100

Initial temperature (K): 293

Output options

Save step: 20

Print step: 20

Constant temperature options

Temperature (K): 1200

Relaxation time: 0.1

☒ Const temperature

Constant pressure options

Px (Mbar): 0

Py (Mbar): 0

Pz (Mbar): 0

Relaxation time: 0.1

Bulk module (Mbar): 0.623

☒ Isotropy ☒ Const pressure

Neighbours list options

Max neighbors: 300

Cutoff factor: 1.2

Hmin: 0.01

Hmax: 0.01

☒ use neighbors list

☐ Stress

☐ Include thermal stress

☐ Restart

UX (eV): 0.295

RX (Å): 4.91

AMX (amu): 28.086

Note: time in reduced units

Reduced time unit= 4.87712e-013 s

OK Cancel Help

The Set parameters for run dialog contains the following fields and buttons:

General options field:

Time step: Allows you to set the time step interval for performing numerical integration of the motion equations. The time step interval will be equal to this factor multiplied on Reduced time unit.

Number steps: Allows you to specify the number of simulation steps.

Initial temperature: Allows you to set the initial temperature of the MD simulation.

Output options field:

Save step: Allows you to specify the frequency for saving of the trajectory files.

Print step: Allows you to specify the frequency for printing and saving other simulation results such as temperature, energy, stresses.

Constant temperature options field:

Const temperature: Check this box to turn on the constant temperature simulation.

Temperature: Allows you to specify the temperature, which will be maintained during the MD simulation.

Relaxation time: Allows specifying the relaxation time constant. The greater value of this constant will require to run more steps to reach the desired temperature. However, the small value of the constant will result in too abrupt changes of the MD quantities. The $100 \times \text{time_step}$ value will be the good value to start.

Constant pressure options field:

Constant pressure: Check this box to turn on the constant pressure simulation.

P_x, P_y, P_z: The Cartesian components of external pressure. The positive value of the pressure will result in compressing the structure. To stretch the structure use the negative value of the pressure.

Isotropy: Check this box to choose isotropic external pressure simulation. For the non-orthogonal lattices you must check this box.

Relaxation time: Allows setting the relaxation time constant. The more value you set to this constant the more steps you need to run to reach the desired value of the pressure. However, the small value of the constant will result in too abrupt changes of the MD quantities. The $100 \times \text{time_step}$ value will be the good value to start.

Bulk module: Allows you to specify the bulk elastic modulus. The value of the bulk elastic modulus should not be necessarily equal to exact real value. In most cases you do not need to change the default value.

Neighbors list options field:

Use Neighbors list: Check this box to use the neighbors list in MD simulation.

Max neighbors: This value is used to build the neighbors list. Increase this value if you receive the error message "the neighbors list too small."

Cutoff factor: All atoms whose separation less than $\text{factor} \times \text{cutoff}$ will be included in the neighbors list. The cutoff is the potential cutoff radius. The factor must be more 1.

Restart: Check this box to continue the previous MD simulation. You can change some parameters of the MD simulation.

Stress: Check this box to turn on the stress calculation during the MD simulation.

Include thermal stress: Check this box to include the velocity dependent part of the stress tensor in the stress calculation.

UX: The reduced factor for energy.

RX: The reduced factor for a distance.

AMX: The reduced factor for a mass.

Reduced time unit: The reduced factor for a time. The real time = reduced time * reduced time unit.

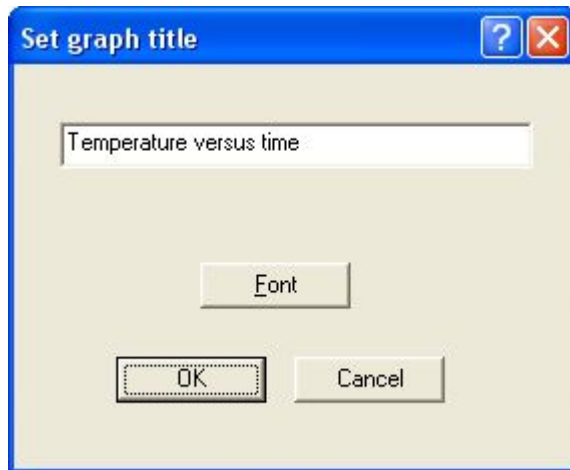
OK: Click this button to start simulation with the current parameters.

Cancel: Click this button to exit the dialog and discard all changes.

4.21 Set graph title dialog box

Path: [Results](#) menu (3.2.8) → one of menu items or

Path: [Graph](#) menu (3.2.9) → one of menu items.



In the text field of this dialog you can enter or change the title of the graph or desired axis.

Font: Click this button to open the font dialog, which allows to change the font type, size and color.

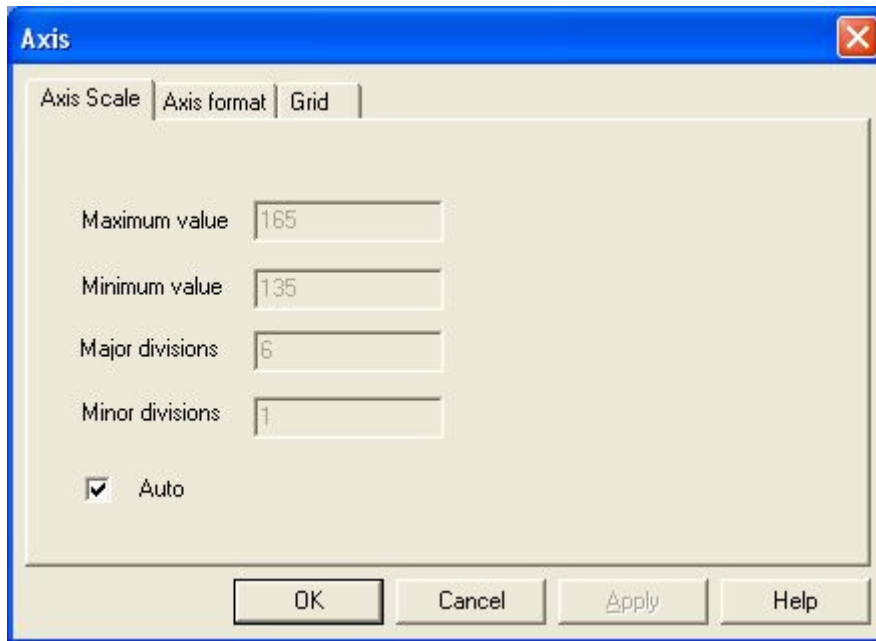
OK: Click this button to apply current settings and close dialog.

Cancel: Click this button to discard all changes and close dialog.

4.22 Axis dialog box

Path: [Results](#) menu (3.2.8) → one of menu items or

Path: [Graph](#) menu (3.2.9) → one of menu items



The Axis dialog allows changing or specifying the axis format, scale and grid.

The Axis dialog contains the following tabs:

[Axis Scale](#) tab (4.22.1)

[Axis Format](#) tab (4.22.2)

[Grid](#) tab (4.22.3)

OK: Click this button to apply current settings and close dialog.

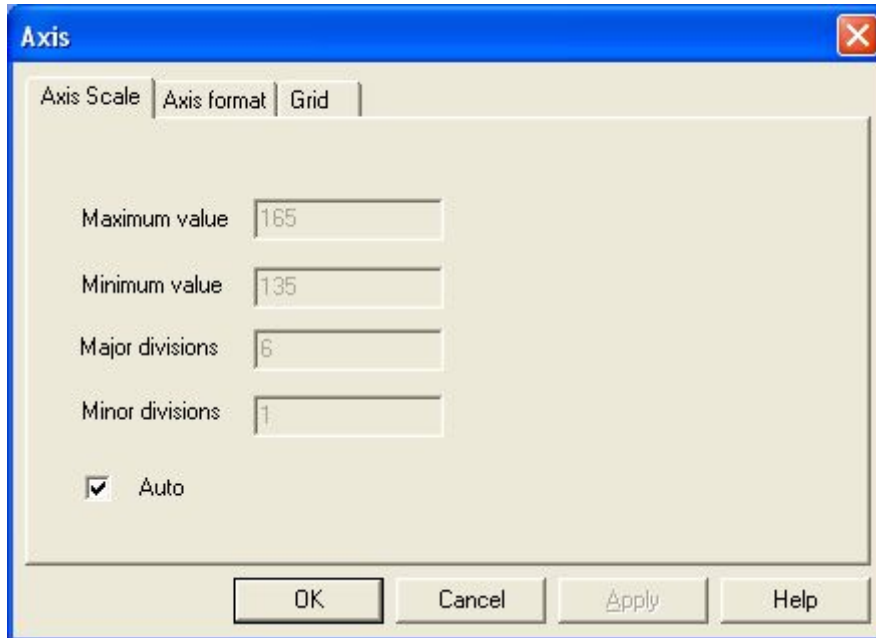
Cancel: Click this button to discard all changes and close dialog.

Apply Now: The same as OK but the dialog will not be closed.

Help: Use this button to get the help about the active tab.

4.22.1 Axis Scale tab

The Axis Scale tab allows changing the axis initial and finite value, the major and minor division scale factor.



The screenshot shows a dialog box titled "Axis" with a blue title bar and a red close button. It has three tabs: "Axis Scale", "Axis format", and "Grid". The "Axis Scale" tab is selected. Inside the tab, there are four input fields: "Maximum value" with the value "165", "Minimum value" with the value "135", "Major divisions" with the value "6", and "Minor divisions" with the value "1". Below these fields is a checkbox labeled "Auto" which is checked. At the bottom of the dialog are four buttons: "OK", "Cancel", "Apply", and "Help".

The Axis Scale tab contains the following fields:

Maximum value: Allows changing the axis finite value.

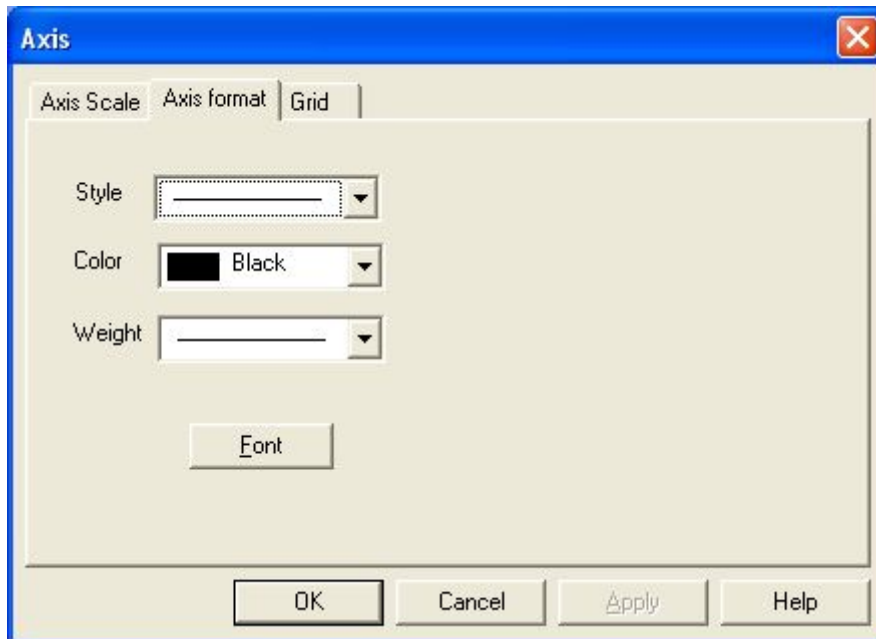
Minimum value: Allows changing the axis initial value.

Major division: Allows changing the major division scale factor.

Minor division: Allows changing the minor division scale factor.

4.22.2 Axis Format tab

The Axis Format tab allows changing the axis style, color and weight.



The Axis Format tab contains the following fields:

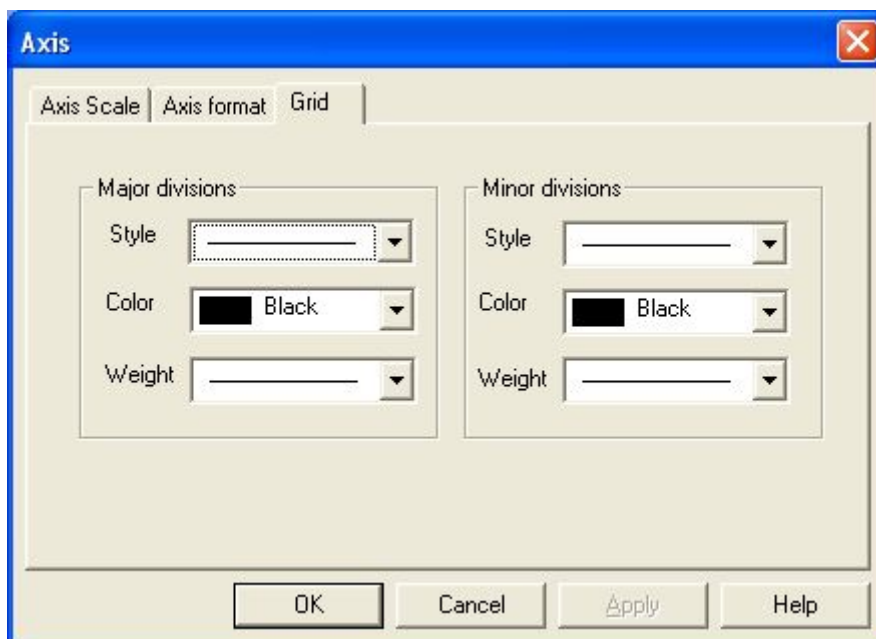
Style: Use this box to select the axis line style from dropdown list.

Color: Use this box to select the axis line color from dropdown list.

Weight: Use this box to select the axis line weight from dropdown list.

4.22.3 Grid tab

The Grid tab allows changing the major or minor grid style, color and weight.



The Grid tab contains the following fields:

Style: Use this box to select the major or minor line style from dropdown list.

Color: Use this box to select the major or minor line color from dropdown list.

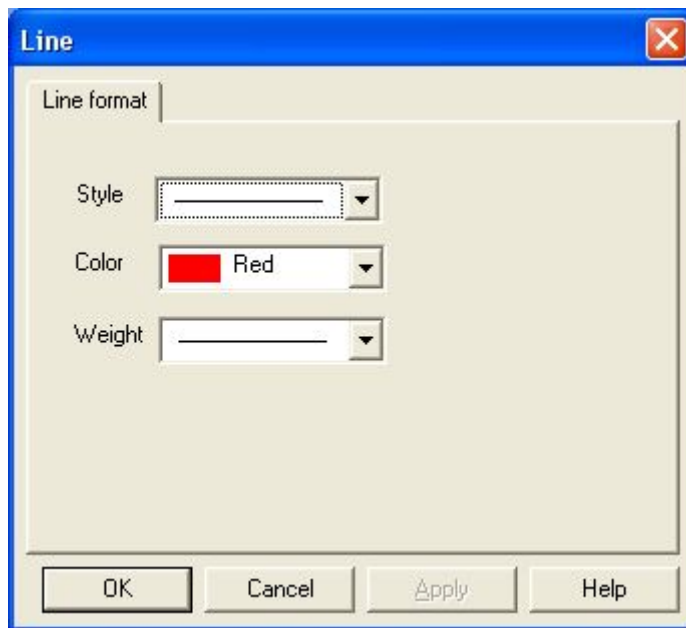
Weight: Use this box to select the major or minor line weight from dropdown list.

4.23 Line Dialog box

Path: [Results](#) menu (3.2.8) → one of menu items or

Path: [Graph](#) menu (3.2.9) → one of menu items.

The Line dialog allows changing the graph line style, color and weight.



Style: Use this box to select the graph line style from dropdown list.

Color: Use this box to select the graph line color from dropdown list.

Weight: Use this box to select the graph line weight from dropdown list.

OK: Click this button to apply current settings and close dialog.

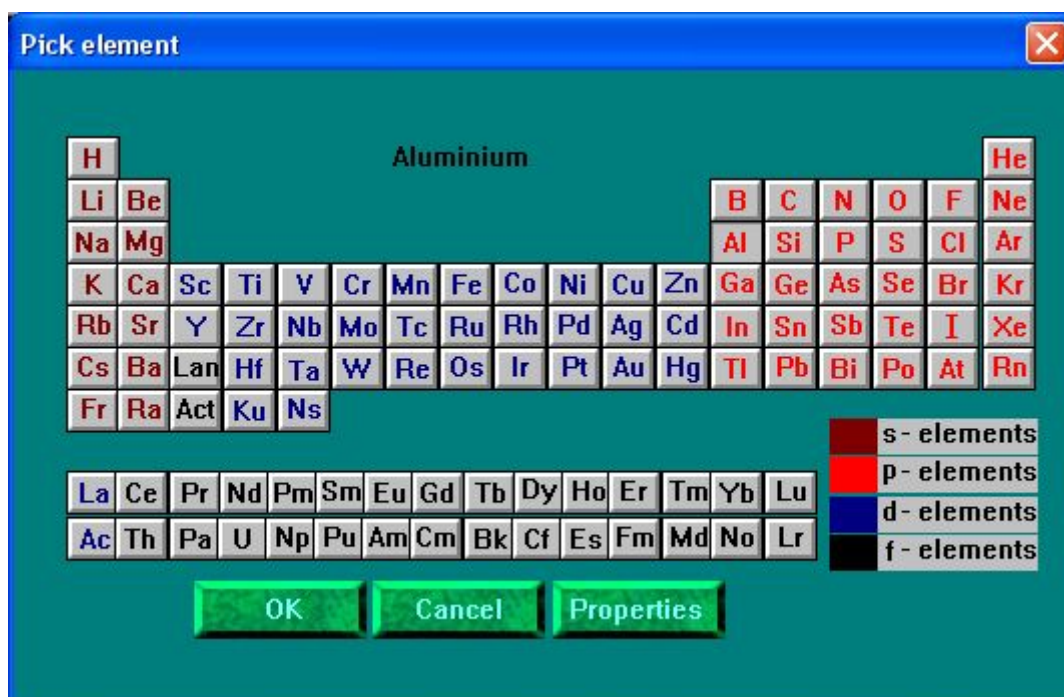
Cancel: Click this button to discard all changes and close dialog.

Apply Now: The same as OK but the dialog will not be closed.

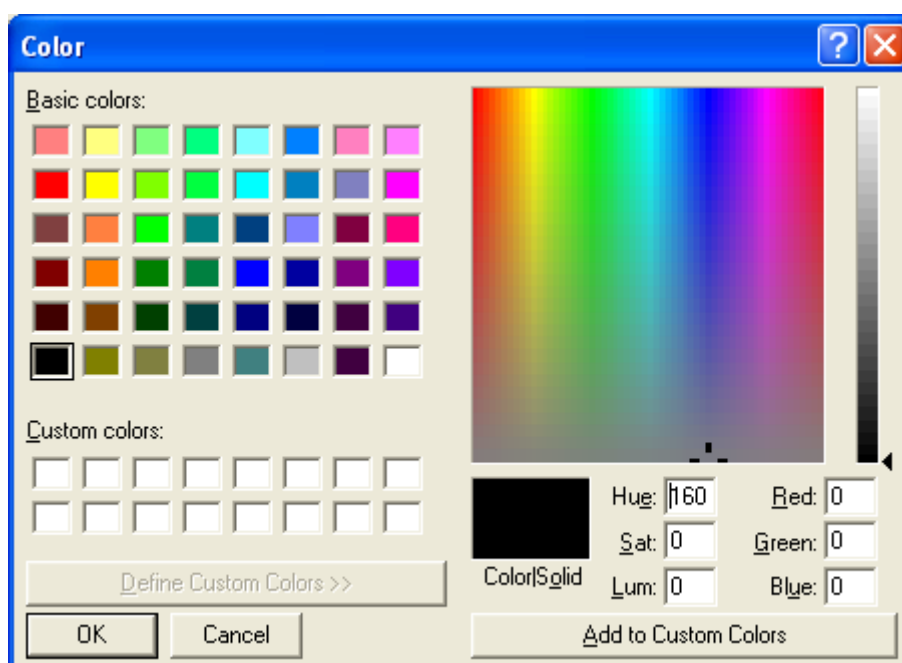
Help: Use this button to get the help.

4.24 Pick element dialog box

Use this dialog to pick the element from the periodic table of elements or to see element's properties. Click on the element symbol button and then click OK button to pick element or click Properties button to see the elements properties.



4.25 Color dialog box




5 Simulation Executing

5.1 Lattice Building

SageMD is a powerful tool for crystal building. Using the different visualization techniques available in **SageMD**, you can create high quality graphics that can be easily pasted into other windows-based software programs or saved as bitmaps.

The next sections describe several ways of the crystal building in **SageMD** code.

5.1.1 Using the SageMD structure database

SageMD has the structure database that contains many different types of structures. You can open the desired structure using the [File](#) menu (3.2.1) or by pressing the  button on the toolbar. A standard Open dialog box is displayed on the screen. Locate the **SageMD** templates directory (usually .../Program Files /SageMD/Template). Open needed subdirectory, select the *.vnd file and click the Open button. The structure will be displayed on your screen. Select [Create](#) (3.2.5.1) from [Lattice](#) menu (3.2.5) and use [Super Cell](#) Tab (4.2.6) in [Lattice builder](#) dialog box (4.2.) to rebuild crystal.

5.1.2 Importing crystals into SageMD from others applications.

You can import the files with format different from **SageMD**. Just open the [File](#) menu (3.2.1) and click on Import item to display on the screen a standard Open dialog box. Choose the required file format from the dropdown list in the bottom of dialog; select the file and press Open button. The crystal will be displayed in the **SageMD** main window.

5.1.3 Building crystal from scratch

There is the consecution of action for building alpha quartz crystal (SiO_2) from scratch:

1. Start **SageMD**.
2. Select New from the [File](#) (3.2.1) menu.
3. Select the and then [Create](#) (3.2.5.1) menu item of [Lattice](#) (3.2.5) menu. The [Lattice Builder](#) dialog (4.2) will be displayed.
4. Under group number enter 154. Make sure that "P3221" is displayed in the [Select space group](#) combo box.
5. Click [Cell](#) tab (4.2.2). Enter $a=4.914$ and $c=5.405$.
6. Click the [Asymmetric Cell](#) tab (4.2.3). Click the [Clear](#) button and then the [Add Atom](#) button. The [Pick element](#) (4.24) dialog box will be displayed.
7. Click the Si button and then [OK](#).
8. In the Edit positions group box on [Asymmetric Cell](#) tab (4.2.3) enter the values: $x=0.4699$ $y=0$ $z=0.6666667$.
9. Click the [Add atom](#) button, choose O and click [OK](#).
10. Enter the position of O atom $x=0.4141$ $y=0.2681$ and $z=0.7854$.
11. Click the [Build unit cell](#) button on [Asymmetric Cell](#) tab (4.2.3) and then the [Unit Cell](#) tab (4.2.5) on [Lattice Builder](#) dialog (4.2). Make sure that the full unit cell contains 9 atoms.
12. Click the [Apply Now](#) button and move the dialog to a screen corner. Use the left mouse button to rotate the lattice and right mouse button to move it.

13. Click the [SuperCell](#) tab (4.2.6) on [Lattice Builder](#) dialog (4.2). Make the number cell in all directions equal to 2. Click the [OK](#) button.

14. From the [File](#) (3.2.1) menu, select the [Save as](#) menu item to save your work. The standard [Save as](#) dialog box will be displayed. Enter "SiO2" as the file name and then choose the directory to save the file and click the [Save](#) button.

5.2 Selecting atoms

Many operations in the **SageMD** operate upon those atoms that are selected in the main window (for example adding volumes, adding a layer of the fixed atoms, deleting atoms and so on). Selected atoms in the 3D view window are displayed in yellow. There are several ways to select one atom or a group of atoms:

- Selecting the individual atom

- Selecting the group of atoms.

- Selecting the spherical, cylindrical or parallelepipedic areas.

- Selecting the atoms according its type.

- Selecting the whole structure and inverting selection.

- Selecting according a plane.

- Selecting the fixed atoms.

5.2.1 Selecting the individual atom

Hold shift key and click atoms to select. The picked atoms become selected, in addition to any atoms already selected. If an atom was already selected it becomes unselected.

5.2.2 Selecting the group of atoms

As an alternative to picking on an individual atom to select it, one or more atoms may be selected graphically by drawing a rectangle with the mouse. All atoms within this region are considered "picked". Hold CTRL key and the left mouse button. Move mouse to draw rectangle around the atoms to select. The starting point of the mouse forms one vertex of the rectangle and the current location of the mouse is the opposite vertex.



5.2.3 Selecting the spherical, cylindrical or parallelepipedic areas

Some tasks for crystal building or interface constructing needs geometrical figures to be selected. The [Select geom...](#) (4.3) dialog box of the [Operations](#) (3.2.6) menu item allows to select areas with spherical, cylindrical or parallelepipedic form.

5.2.4 Selecting the atoms in concordance with its type.

If you want to select all the same type atoms of the current crystal structure use the [Select type](#) (4.4) dialog box of the [Operations](#) (3.2.6) menu item.

5.2.5 Selecting the whole structure and inverting selection.

You can select all atoms by pressing the CTRL+A keyboard buttons, or choose [Select all](#) (3.2.6.2) menu item of the [Operations](#) (3.2.6) menu, or click once  button on the toolbar. Also you can invert your selection by pressing ALT+A, or choosing [Select invert](#) (3.2.6.5) menu item of the [Operations](#) (3.2.6) menu or clicking once  button on the toolbar.

5.5.6 Selecting according a plane.

Sometimes it is necessary to select some region that should be limited by a plane. With the help of the [Select by plane](#) dialog box (4.5) you can specify a plane that divides the structure into two parts. One of the parts will be selected after you click on the [Select](#) button of this dialog.

5.5.7 Selecting fixed atoms.


Sometimes it is necessary “to freeze” the group of the selected atoms in the current MD simulation. The coordinates of these atoms will not be changed during the whole simulation. Select requisite group of atoms and click [Add fixed atoms](#) menu item (3.2.7.10) in the [Task](#) menu (3.2.7).

5.3 Setting the parameters for the MD simulation and run simulation

1. Build lattice by one of the ways, described in the section 5.1.
2. Use [Display parameters](#) (4.1) dialog to change atoms colors, sizes, rendering quality and build atom bonds if it is necessary. **Menu path:** [Display](#) → [Parameters](#).
3. Use [Set potential](#) (4.14) dialog to set interatomic potential for atoms. You can implement your own pair potential. To do it you need prepare your own potential file. The format of the file is [EAM potential file format](#) (2.2.4). Only the pair section must be presented in this case. Choose EAM potential in the [Set potential](#) (4.14) dialog box and specify your file as EAM potential file. **Menu path:** [Tasks](#) → [Set potential](#).
3. Set boundary conditions. The periodic boundary conditions in all direction are default settings. Use [Set boundary conditions](#) (4.17) dialog to change default settings. **Menu path:** [Tasks](#) → [Boundary condition](#).
4. If you wish calculate the RDF (Radial Distribution Function) or MSD (Mean Square Displacement) you need to set volumes. Also, you must set volumes if you wish monitoring the temperature and stresses in some part of the simulation cell. Select atoms, which you wish to insert into a volume and click [Set volumes](#) menu item (3.2.7.5) from [Tasks](#) (3.2.7) menu to display [Set volumes](#) dialog box (4.17), which allows you to set the volume parameters. To calculate RDF and MSD for the whole simulation cell select all atoms as the volume. You can create up to 20 volumes. **Menu path:** [Tasks](#) → [Set volumes](#).
5. Use [Ewald sum parameters](#) (4.15) dialog box if your pair potential has Coulomb item. Also, you can use qEq model in this case. However, the number of atoms must be less then 600 to use qEq model. **Menu path:** [Tasks](#) → [Ewald sum](#) and [Tasks](#) → [qEq](#).
6. Optionally, you can fix the selected atoms positions during MD simulation. The positions of the fixed atoms are not updated during the MD simulation and their velocities will be set to 0. **Menu path:** [Tasks](#) → [Add fixed atoms](#).
7. Use [Set parameters for run](#) (4.20) dialog to set other parameters and start the MD simulation. **Menu path:** [Tasks](#) → [Run](#).
8. Click [OK](#) button to close the dialog. The MD simulation script file will be displayed. **Close it** to start simulation.

5.4 Monitoring the simulation

After starting the MD simulation click the [Graph](#) menu (3.2.9) and select [Temperature](#) menu item, or [Volumes Temp](#) menu item if any volumes were selected. You may observe representation of selected quantity on graph.

When the simulation is done click the  icon on the toolbar.

5.5 Viewing the results

Use some of menu items of the [Results](#) menu (3.2.8) in concordance with your task to see graphs. Use [Tile vertically](#) menu item of the [Windows](#) menu to see all graphs simultaneously. To scale graphs double click on the desired axis. Double click on the line to change line properties. Double click on titles to change the title text and font.

You can copy the graphs data to the MS Excel. Activate the graph window and use Ctrl + C keyboard shortcut to copy the graph to the clipboard. Start MS Excel and use Ctrl + V shortcut to paste the graph data on MS Excel sheet. To paste the graph to MS Word use “Paste special” command from the “Edit” menu of this application. The print command will be realized soon.

6 Sources of information – Libraries and Databases

6.1 Database on structures

SageMD database on structures represent the library of ready for use files (with extension .vnd) that contains unit cell structures for many different elements and crystalline materials. This library is located in **SageMD** templates directory (usually .../Program Files /SageMD/Template). See in section [5.1.1](#) how to build lattice, using the **SageMD** structure database.

You may to supplement database by your own unit cell structures. See in section [5.1.3](#) how to build unit cell structure, using the **SageMD**.

6.2 Database on potential parameters

Excuse, it's not ready now.

7 Tutorial. Melting of the Al crystal

The eam_al.vnd file is the ready for use the project file for this tutorial. You can find it in the "Template" subdirectory of the **SageMD** installation directory. However, you need to correct the path to al.pot file. In this tutorial the path is E:\Program Files\SageMD\EAM\al.pot. If during installation you choose the default path then you need only to change the drive letter. Save the project file in the new directory before you start the simulation. All output files will be created in the directory where you saved the project file.

7.1 Building of the Al crystal

Double-click the **SageMd** icon on your desktop.

Select [Open...](#) from the [File](#) menu (3.2.1). The [Open file](#) dialog will be displayed.

Locate the **SageMD** templates directory. (Usually .../Program Files /**SageMD**/Template). Open the "elements" subdirectory, select the Al.vnd file and click the [Open](#) button. The unit cell of the Al structure will be displayed.

Click the  icon on the toolbar. The [Lattice builder](#) dialog box (4.2) will be displayed.

Click the [SuperCell](#) tab (4.2.6). Make the number of unit cell in all directions equals 5 and click the [OK](#) button.

From the [File](#) menu (3.2.1), select the [Save as](#) menu item. The [Save as](#) dialog will be displayed. Use it to save your work. It is recommended you save the file in new directory because of all input and output files will be located here.

7.2 Setting the parameters for the MD simulation

7.2.1 Setting the potential parameters

From the [Tasks](#) menu (3.2.7), select the [Set potential](#) menu item (3.2.7.2). The [Set potential](#) dialog box (4.14) will be displayed.

From the [Potential](#) dropdown list select "EAM" (Embedded Atom Method) and click the [Poten file](#) button. The [Set EAM potential file](#) dialog will be displayed.

Type the full path to the al.pot file or use [Browse](#) button to locate this file. (Usually .../Program Files/ SageMD/EAM/al.pot).

Click [OK](#) button to close [Set EAM potential file](#) dialog box and then [OK](#) button to close [Set potential](#) dialog box.

7.2.2 Setting parameters for RDF and MSD calculation.

We wish to run the 3000 steps of the MD simulation. The RDF function will be calculated using the 500 last steps. The MSD we will calculate using all steps. We wish to calculate the RDF function and MSD using all atoms of the crystal. Thus, we need to select all atoms. Hold Ctrl and press C keys to select all atoms.

From the [Tasks](#) menu (3.2.7), select the [Set volumes](#) menu item (3.2.7.5). The [Set volumes](#) dialog box (4.17) will be displayed.

Click the [Add volume](#) button.

Click "NoName" and type the volume name (for example Box1 or Box1.txt).

Click the "+" mark to expand the list tree.

Click the "+" mark to expand the RDF tree.

Click the "+" mark to expand the [first_step](#) tree.

Click the "1" box to select it, then click it again to edit.

Type 2500 and click the "+" mark to expand [last_step](#) tree.

Click the "1" box to select it, then click it again to edit.

Type 3000 and click the "+" mark to expand [Msd](#) tree.

Set the [last_step](#) to 3000 and click [Close](#) button to close the [Set volumes](#) dialog box.

7.2.3 Setting the general parameters.

From the [Tasks](#) menu (3.2.7), select [Run](#) menu item (3.2.7.8). The [Setting parameters for run](#) dialog box (4.20) will be displayed.

Type 3000 in the [number steps](#) box.

Type 10 in the [Save step](#) box to set frequency for saving the trajectory file.

Type 10 in the [Print step](#) box to set frequency for saving the other output files.

Check the [Stress](#) checkbox to output stresses during the MD simulation.

Check the [Const temperature](#) checkbox and type 1500 in the [Temperature](#) and 1 in the [Relaxation time](#) boxes.


Check the [Const pressure](#) checkbox and type 1 in the [Relaxation time](#) box.

Click [OK](#) button to close the dialog. The MD simulation script file will be displayed. **Close it** to start simulation.

7.3 Monitoring the simulation

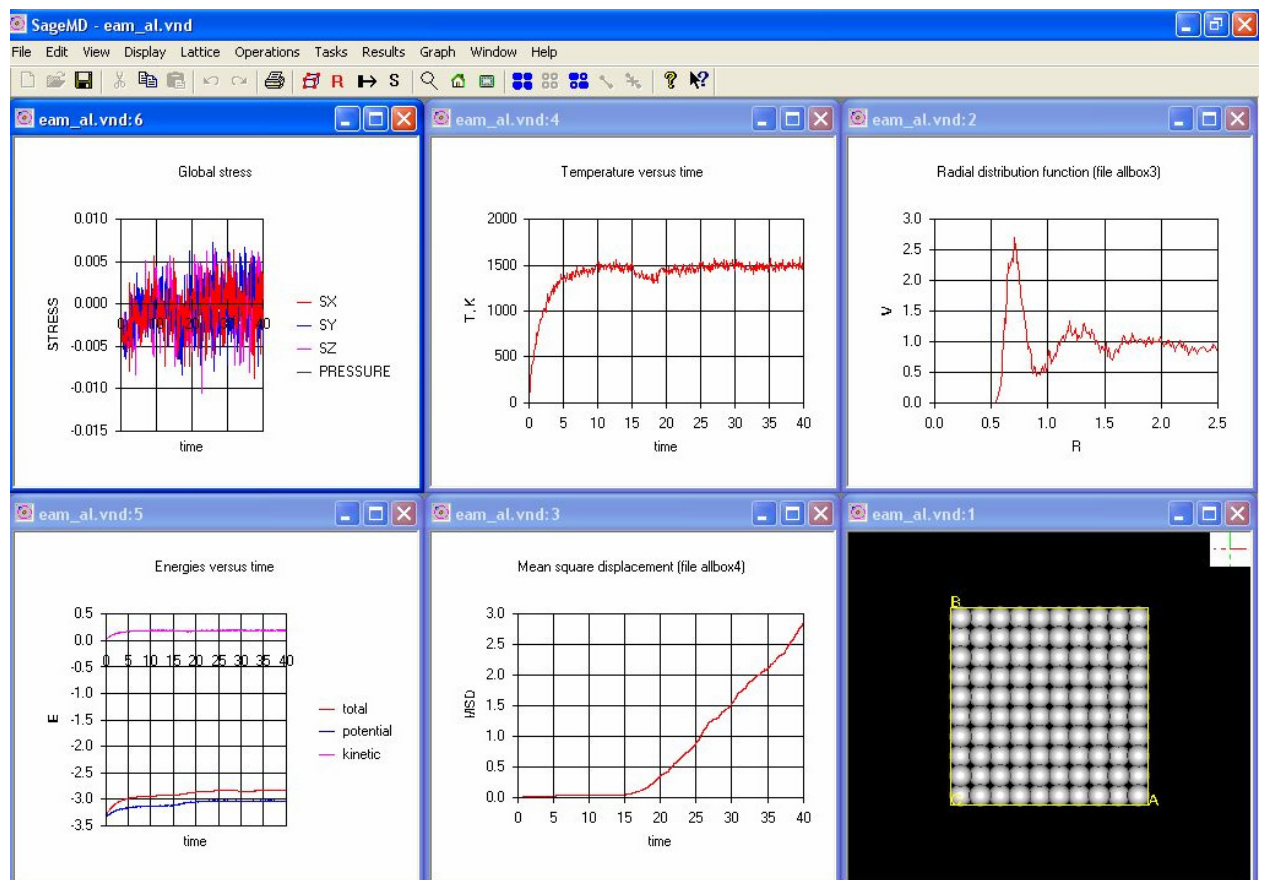
After starting the MD simulation click the [Graph](#) menu (3.2.9) and select [Temperature](#) menu item.

From the [Window](#) menu select [Tile vertically](#) menu item. You can see the temperature graph and the aluminum structure simultaneously.

When the simulation is done click the  icon on the toolbar.

7.4 Viewing the results

Use [Graph RDF](#), [Graph MSD](#), [Graph temp](#), [Graph energy](#) and [Graph stress](#) menu items of the [Results](#) menu (3.2.8) to see graphs. Use [Tile vertically](#) menu item of the [Windows](#) menu to see all graphs simultaneously.



8 Final Results – Documents and Files

Excuse, it's not ready now.

9 How to work with 3D graphics



You can always change the display style of a current structure. Using the options of the Display parameters dialog, you can control several stylistic features of the structures displayed in the main window of the **SageMD** code. Some of the characteristics you control in the Display parameters dialog are:

- The rendering style, size and color of the atomistic structure.
- Various parameters of the bonds building.
- The color of the background and selected atoms.
- The style and form of the contour around the lattice.
- The style of viewing atomic structure (orthogonal or perspective).

9.1 The rendering style, size and color of the atomistic structure

The [Atom](#) tab (4.1.1) of the [Display parameters](#) dialog box (4.1) controls the graphical representation of atoms. Here you can change the atomic sizes, colors and the quality of the rendering of the OpenGL graphics. For example, to change the atoms colors just click on the color you want to change. The [Color](#) dialog box (4.25) will be displayed. Pick the desired color and click **OK** button to close the [Color](#) dialog box. All the structure elements in **SageMD** are given a default color, usually defined by the type of atomic element. But sometimes it is useful to give a custom color to the chosen element.

9.2 Various parameters of the bonds building.

Use [Bond](#) tab (4.1.2) on the [Display parameters](#) dialog box (4.1) to build the atoms bonds, change bonds radius, show or hide the bonds image. This tab allows to change parameters for the whole structure. But if you wish to build several bonds between some atoms you must carry out the following actions: First, make sure that in the [Bond](#) tab (4.1.2) of the [Display parameters](#) dialog (4.1) the [Auto rebuild](#) check box is unchecked and the [Show bonds](#) check box is checked. Then click the  button on the toolbar. Hold the shift key and click the two atoms whose bond you wish to build. If you want to remove bond just click the  button in the toolbar and select this atoms. Also you can use [Add bonds](#) (3.2.6.19) and [Remove bonds](#) (3.2.6.20) menu items in the [Operations](#) menu (3.2.6).

9.3 The color of the background and selected atoms.

The default color of the background is black. As for selected atoms it is yellow. But you can change the color manually (for example before capturing and importing atomic structure 3D view image). You can change these parameters from the [Misc](#) tab (4.1.3) of the [Display parameters](#) dialog box (4.1).

9.4 The style and form of the contour around the lattice. The style of viewing atomic structure (orthogonal or perspective).

These two characteristics can be also controlled from the [Misk](#) tab (4.1.3) of the [Display parameters](#) dialog box (4.1).

Just choose wanted projection in the projection field. Depending on you choice the projection will be orthogonal or perspective. Also you can specify how the contour around the crystal will be displayed. Select Hide to hide the contour image. Select Unit cell to display the contour around the unit cell. Select lattice to display the contour around the whole crystal

10 Questions and Answers...

A1. How can I select atoms?

Hold shift key and click atoms to select.

Hold ctrl key and the left mouse button. Move mouse to draw rectangle around atoms to select.

From the [Operation](#) menu (3.2.6), select the [Select geom...](#) (3.2.6.1) menu item.

From the [Operation](#) menu (3.2.6), select the [Select type](#) menu item (3.2.6.4).

To select all atoms use the ctrl+A keyboard shortcut.

A2. How can I fit the lattice image to the display screen?

Press the spacebar.

A3. How can I see the coordinates of the atoms?

From the [Operation](#) menu (3.2.6), select the [Edit atoms](#) menu item (3.2.6.18) to display the [List and edit atom position](#) dialog box (4.12).

Select the atom whose position you wish to see.

The atom coordinates will be displayed in the "Edit position" group box.

A4. How can I change the atom position and/or atom type?

From the [Operation](#) menu (3.2.6), select the [Edit atoms](#) menu item (3.2.6.18) to display the [List and edit atom position](#) dialog box (4.12).

Select the atom whose position you wish to change.

The atom coordinates will be displayed in the [Edit position](#) group box.

Enter the new atom position coordinates and click the [Apply](#) button.

To change the atom type use the combo box under the [Change atom](#) group box.

A5. How can I measure the distance between the atoms?

From the [Operation](#) menu (3.2.6), select the [Check lattice](#) menu item (3.2.6.16) to display the [Check lattice](#) dialog box (4.10).

Hold the shift key and click the two atoms whose separation you wish to measure.

A6. How can I measure the angles between the atoms?

From the [Operation](#) menu (3.2.6), select the [Check lattice](#) menu item (3.2.6.16) to display the [Check lattice](#) dialog box (4.10).

Click the [Check angles](#) tab (4.10.2). Make sure that the Torsion angles check box is not checked.

Hold the shift key and click the three atoms to measure the angle between them. At first you need to click the atom, which is the vertex of the angle.

A7. How can I measure the torsion angles?

From the [Operation](#) menu (3.2.6), select the [Check lattice](#) menu item (3.2.6.16) to

display [Check lattice](#) dialog box (4.10).
Click the [Check angles](#) tab (4.10.2). Make sure the [Torsion angles](#) check box is checked.
Hold the shift key and click the two atoms B and C whose torsion angle you wish to measure.
Then click the two atoms A and D, which are bonded to B and C respectively.

A8. How can I paste the lattice image into MS Word document?

From the [Edit](#) menu (3.2.2), select the [Capture image](#) menu item.
Hold the left mouse button and move mouse to draw rectangle around the lattice.
After releasing the mouse button the lattice image will be copied to the clipboard.
After that you can paste the image in such applications as Word, Power Point, Excel, Paint using “Paste” command from “Edit” menu of this applications.

A9. Can I save the lattice image in the file?

Yes, you can save the lattice image as the bitmap (bmp) file.
From the [Edit](#) menu (3.2.2), select the [Capture image to file](#) menu item.
Hold the left mouse button and move mouse to draw rectangle around the lattice.
After releasing the mouse button the [Save as](#) dialog box will be displayed.
Use this dialog to save the image.

A10. Can I print the lattice image?

No, you cannot. This feature will be implemented soon. However, you can paste the lattice image in the MS Word document and print it.

A11. How can I change the atoms colors?

From the [Display](#) menu (3.2.4) select the [Parameters](#) menu item (3.2.4.1).
The [Atom](#) tab (4.1.1) of the [Display parameters](#) dialog box (4.1) will be displayed.
Click on the color you wish to change. The [Color](#) dialog box (4.25) will be displayed.
Choose color and click [OK](#) button.

A12. How can I change the atoms sizes?

From the [Display](#) menu (3.2.4) select the [Parameters](#) menu item (3.2.4.1).
The [Atom](#) tab (4.1.1) of the [Display parameters](#) dialog box (4.1) will be displayed.
Click the size you wish to change. The [Change ball size](#) dialog will be displayed.
Type the new size and click [OK](#) button.

A13. How can I build the bonds?


From the [Display](#) menu (3.2.4) select the [Parameters](#) menu item (3.2.4.1).
Click the [Bond](#) tab (4.1.2). If the [min factor](#) and [max factor](#) have values equals to zero make it equals to 0.6 and 1.1 respectively.

Click Build button. If no bonds are displayed you need to increase the value of the max factor. Make sure the Show bonds and Auto rebuild check boxes are checked.

A14. How can I add/remove the bonds manually?

Make sure that  (add bond) and  (remove bond) toolbar icons are available.

If it is not then from the Display menu (3.2.4) select the Parameters menu item (3.2.4.1). Click the Bond tab (4.1.2) and uncheck the Auto rebuild check box. Make sure that the Show bonds check box is checked.

Click the  icon on the toolbar to build the bonds.

Hold the shift key and click the two atoms whose bond you wish to build.

Click the  icon on the toolbar to remove the bonds.

Hold the shift key and click the bond you wish to remove.

A15. How can I change the background color?

From the "Display" menu select the Parameters menu item (3.2.4.1). Click Misc tab. Click the background color. The "Choose color" dialog will be displayed. Choose color and click "OK" button.

A16. How can I hide/show the contour around the lattice?

From the Display menu (3.2.4) menu select the "Parameters..." menu item. Click "Misc" tab (4.1.3).

Check the Hide radio button to hide the contour.

Check the Unit cell radio button to draw contour around the unit cell.

Check the lattice radio button to draw contour around the crystal.

A17. Can I paste the atoms positions into the Notepad or Word documents?

Yes, you can. Select the atoms whose positions you wish to paste. You can select all atoms.

From the Edit menu (3.2.2) select Copy or use the ctrl+C keyboard shortcut to copy the atoms positions to the clipboard. After that you can paste the positions into the applications using their the "Paste" command from the "Edit" menu. The following example is the pasting of the SiC cubic unit cell into MS Word document.

```
NumberAtoms=8
Si 0 0 0
Si 0 2.174 2.174
Si 2.174 0 2.174
Si 2.174 2.174 0
C 1.087 1.087 1.087
C 1.087 3.261 3.261
C 3.261 3.261 1.087
C 3.261 1.087 3.261
```

If you place the text in such format to the clipboard then you can paste

these atoms into the **SageMD** document.

A18. How can I delete atoms?

Select the atoms to delete. Press the Del key.
To delete all atoms use the ctrl+Del keyboard shortcut.

A19. How can I rotate the lattice image?

Hold the left mouse button and move the mouse to rotate the lattice image.

A20. How can I move the lattice image?

Hold the right mouse button and move the mouse to move the lattice image.

A21. How can I export the lattice to Siesta code?

From the [File](#) menu (3.2.1) select the Export menu item. The Save as dialog will be displayed.

Select the fdf extension in the Save as type box. Type the file name in the File name.

box and save the file. The following example shows the .fdf file generated by SageMD.

```
NumberOfAtoms 9
```

```
NumberOfSpecies 2
```

```
%block Chemical_Species_label
```

```
1 14 Si
```

```
2 8 O
```

```
%endblock Chemical_Species_label
```

```
LatticeConstant 1 Ang
```

```
%block LatticeVectors
```

```
4.2522 -2.455 0
```

```
0 4.91 0
```

```
0 0 5.402
```

```
%endblock LatticeVectors
```

```
AtomicCoordinatesFormat ScaledCartesian
```

```
%block AtomicCoordinatesAndAtomicSpecies
```

```
2.0444 1.1803 0.0000 1
```

```
0.6386 1.6669 0.6293 2
```

```
3.1279 1.0685 1.1713 2
```

```
0.0000 2.5494 1.8007 1
```

```
1.1243 3.5235 2.4300 2
```

```
3.6136 -0.7881 2.9720 2
```

```
2.2078 -1.2747 3.6013 1
```

```
2.4893 2.1746 4.2307 2
```

```
1.7629 -0.2804 4.7727 2
```

```
%endblock AtomicCoordinatesAndAtomicSpecies
```

```
##%include default.fdf
```

Use "include" directives to include the other Siesta data.

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