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Comparison of MEAM-2NN and Sutton-Chen Mathematical Models for Computing Mechanical Properties of Binary Alloys of $Cu - Ag$

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***Abstract*:** The computations of the mechanical properties of the pure metals Cu, Ag and their alloys $AgCu_3$ and $CuAg_3$ are presented using the Modified Embedded Atom Method Second Nearest-Neighbour (MEAM-2NN) and Sutton-Chen (SC) mathematical models. These inter-atomic potentials are frequently used to model the energy of atomic interactions in metals and their alloys. The comparison is made to see how well these semi-empirical atomic potentials perform in terms of computing mechanical properties and the dynamic memory needed by the models. The result of our work could be used as a reference point in selecting semi-empirical potentials to model mechanical properties of metals and their alloys. The general utility lattice program (GULP) was used to model the mechanical characteristics of the metals [1]. The time taken to complete the simulations using Sutton-Chen (SC) potential is much lower than when using MEAM-2NN model. The values of the mechanical properties of the pure metals Cu and Ag obtained using the MEAM-2NN are much closer to the experimental values than the values obtained using SC potential. The peak dynamic memory used while using MEAM-2NN inter-atomic potential is much higher than when SC model is utilized in the simulation process[1].

***Keywords*:** Inter-atomic potential, dynamic memory, elastic constant, elastic modulus, acoustic velocity.

1. INTRODUCTION

The force field or interatomic potential is at the heart of atomistic simulations like Geometry Optimization, Molecular Dynamics (MD), or Monte Carlo. They specify how atoms interact in a system, and the correctness of the results is dependent on which potentials are chosen to model the energy of atomic interactions. It is necessary to select appropriate interatomic semi-empirical potentials in order to mimic the desired attributes of the materials under inquiry. There are a number of interatomic potentials that can be used to model the energy of atomic interactions in metals and their alloys. The challenging task is how to choose the potential that represent the interactions among the atoms constituting the material with reasonable precision. The $MEAM-2NN$ and the Sutton-Chen semi-empirical potentials are some of the frequently used models in simulation of metals and their alloys. It is self-evident that one interatomic model may be better at forecasting some attributes while the other method is better at calculating other material properties. It's also worth mentioning that the models' performance may be element-dependent. To evaluate the advantages of one model over the other, a comparison of the methods for forecasting the desired properties of the materials is required.

Because of the widespread availability of computer computing capabilities, scientists and industry specialists have been able to develop higher-performance materials that can be used in chemical industries and as low-weight, high-strength structural materials [2]. The composites of $Cu-Ag$ alloys find wide range applications in electricity due to their high strength and electrical conductivity [3].

Here, we simulated Cu, $AgCu_3$, $CuAg_3$ and Ag using the two semi-empirical interatomic potentials. The purpose of these simulations is to compare the performance of the potentials in predicting the mechanical properties such as elastic constants, bulk and shear moduli, and acoustic velocities of the metals and their alloys. The study's findings will reveal the relative advantages of each interatomic potential. This will aid in the selection of mathematical models for the energy of atomic interactions in metals and alloys.

2. MATHEMATICAL MODELS

One of the challenges in computer simulation methods is the task of finding inter-atomic potential that accurately models the interaction among the atoms that constitute the material [4]. The commonly used potentials for modeling atomic interaction in face centered metals and alloys are the Sutton-Chen interatomic potential and the Modified Embedded Atom Method (MEAM).

The total potential energy of interatomic interactions in the framework of the Sutton-Chen model is expressed as follows [5]:

$$U_{\text{tot}} = \sum_i U_i = \sum_i \left[\frac{1}{2} \sum_{i \neq j} \epsilon_{ij} \left(\frac{a_{ij}}{r_{ij}} \right)^{n_{ij}} - c_i \epsilon_{ij} \left(\sum_{j \neq i} \left(\frac{a_{ij}}{r_{ij}} \right)^{m_{ij}} \right)^{\frac{1}{2}} \right] \quad (1)$$

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where the first term in equation (1) represents a pairwise long-range van der Walls interaction between the i and j atomic cores separated by a distance r_{ij}. The second term introduces the many body cohesive term in relation to the atom i while the square root term describes a many body component into the energy summation. In equation (1), r_{ij} is the separation distance between the atoms i and j, a is a lattice parameter with dimension of length, $c > 0$ is a dimensionless parameter that scales the cohesive term in relation to the repulsive term, ϵ is a energy parameter, n and m are integer material parameters with the property $n > m$. The SC potential could be extended to model alloys using the combination rules for the parameters [5]:

$$\epsilon_{ij} = \sqrt{\epsilon_i \epsilon_j}, a_{ij} = \frac{a_i + a_j}{2}, \\ m_{ij} = \frac{m_i + m_j}{2}, n_{ij} = \frac{n_i + n_j}{2}. \tag{2}$$

Table 1. The parameters of the Sutton-Chen potential for the metals Cu and Ag [6].

Metal	m	n	ϵ (eV)	c	a (Å)
Cu	6	9	1.2382×10^{-2}	39.432	3.6100
Ag	6	12	2.5415×10^{-3}	144. 41	4.0900

The modified embedded atom method (MEAM) potential was written in such away that it would describe metals and materials with covalent bonds having one function expression [7, 8]. This potential models well interatomic interactions in metallic crystals with face centred cubic(fcc), body centred cubic (bcc) and hexagonal close packed (hcp) structures. In the original formalism of MEAM, only the interactions of the first nearest neighbours denote as 1NN were taken into considerations [9]. This was extended to include the second nearest neighbour (2NN) interactions by Lee and Baskes [10].

In the MEAM mathematical formalism the total energy of the system is given as [11]:

$$E_{tot} = \sum_i \left[F_i(\bar{\rho}_i) + \frac{1}{2} \sum_{i \neq j} S_{ij} \phi_{ij}(R_{ij}) \right], \tag{3}$$

where F_i is the embedding function, $\bar{\rho}_i$ is the background electron density at site i, S_{ij} is a multi-body screening factor and $\phi_{ij}(R_{ij})$ is the pair interaction between atoms i and j at a distance R_{ij}. The embedding function F_i is expressed as follows [11]:

$$F(\bar{\rho}) = AE_c \left(\frac{\bar{\rho}}{\bar{\rho}^0} \right) \ln \left(\frac{\bar{\rho}}{\bar{\rho}^0} \right), \tag{4}$$

where A is an adjustable parameter, E_c is the sublimation energy and $\bar{\rho}^0$ is the background electron density for a reference structure. The detailed descriptions of the MEAM-1NN and MEAM-2NN can be found [12].

3. MECHANICAL PROPERTIES OF THE METALS

For a general 3-D material there are six components of stress and a corresponding six components of strain. Applying Hooke's law, the relation between stress and strain is expressed as [13]:

$$\sigma_i = C_{ij} \epsilon_j, \tag{5}$$

where C is elastic constant, σ is stress and ϵ is strain. For evaluating elastic constants, GULP has the computing resources. Atomic coordinates determine the potential energy. Elastic constants are obtained by taking the second derivative of the potential energy function in terms of strain [1]:

$$C_{ij} = \frac{1}{V} \frac{\partial^2 U}{\partial \epsilon_i \partial \epsilon_j}, \tag{6}$$

where C_{ij} is a component of the stiffness matrix C, U is the energy expression, V is the volume of the unit cell, ϵ_i and ϵ_j are strain. For fcc cubic crystals the only unique elements are the elastic constants C_{11}, C_{12} and C_{44}. In terms of the interatomic potentials, the equation used to compute the values for these independent elastic constants can be expressed as follows [14]:

$$C_{11} = \frac{1}{V} \frac{\partial^2 U}{\partial \epsilon_{11}^2}; C_{12} = \frac{1}{V} \frac{\partial^2 U}{\partial \epsilon_{11} \partial \epsilon_{12}}; C_{44} = \frac{1}{4V} \frac{\partial^2 U}{\partial \epsilon_{12}^2}. \tag{7}$$

For isotropic polycrystalline materials, the bulk modulus (B) and shear modulus (G) can be estimated from elastic constants C_{ij} [15]. In computer simulations, the bulk and shear moduli are computed from elastic constants. One of the most widely used methods to estimate the elastic characteristics of polycrystalline materials is the averaging of the single crystal elastic moduli, known as the Voigt (V), Reuss (R) and Hill (H)[15]. Hill showed that the Voigt approximation leads to overestimated values of the elastic moduli, while the Reuss approximation underestimated the values [16], and recommended to take the arithmetic mean of value of these approximations[17]. The formulas for estimation of bulk and shear moduli due to the Voigt(V) and Ruess (R) approximations are given as follows:

$$B_V = B_R = \frac{1}{3}(C_{11} + 2C_{12}); \tag{8}$$

$$G_V = \frac{1}{5}(C_{11} - C_{12} + 3C_{44}); \tag{9}$$

$$G_R = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C - 11 - C_{12})}. \tag{10}$$

The bulk and shear moduli of metals and alloys were calculated using the Hill(H) approximations. For fcc crystal structures, $B_H = B_V = B_R$, whereas the Hill's approximation value for shear modulus is computed using the formula below [15]:

$$G_H = \frac{G_V + G_R}{2}. \tag{11}$$

Acoustic velocity, often known as sound speed, is the rate at which a tiny disturbance propagates across a specific material medium. Acoustic velocity measurements provide information on the properties of both artificial and natural materials. They're crucial when it comes to understanding seismic data [18]. Many fundamental solid-state parameters, such as acoustic velocity, thermal conductivity, Debye temperature and so on, are strongly related to elastic properties [19]. The average acoustic velocity (V_m) in polycrystalline materials is linked to the fundamental material parameter Debye temperature and is calculated as follows [20]:

$$V_m = \left[\frac{1}{3}\left(\frac{2}{v_t^3} + \frac{1}{v_l^3}\right)\right]^{-1/3} \tag{12}$$

where the material's transverse and longitudinal velocities are V_t and V_l, respectively. These values are calculated using the formulas below, which are based on the bulk, shear moduli, and density (ρ) values of metals and alloys [21]:

$$v_t = \left(\frac{G_H}{\rho}\right)^{1/2} \quad and \quad v_l = \left(\frac{3B + 4G_H}{3\rho}\right)^{1/2}. \tag{13}$$

4. SIMULATION OF THE MECHANICAL PROPERTIES

GULP was used to run the simulation in this case. General Utility Lattice Program (GULP) is an acronym for general utility lattice program. This computer code can run simulations in a range of dimensions, from 0-D (molecules and clusters) to 3-D (periodic solids), both with and without boundary conditions [1].

The metals Cu and Ag have face centred cubic (fcc) [22] while the alloys $CuAg_3$ and $AgCu_3$ have $L1_2$ (see Figure 1) [2] crystal structure.

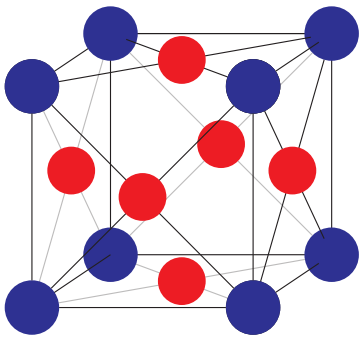

Figure 1. $L1_2$ crystal lattice structure

The coordinates of the atoms utilized in simulation are built using the unit cell, which is the most basic elementary cell. For example, the unit cell for the alloy $AgCu_3$ has the following basis vectors: Ag: $a(0.0, 0.0, 0.0)$; Cu: $a(0.5, 0.5, 0.0)$; Cu: $a(0.0, 0.5, 0.5)$; and Cu: $a(0.5, 0.0, 0.5)$. Here a is the edge of an elementary cube. By translating the unit cell in three dimensions, a cube of 27 unit cells ($3 \times 3 \times 3 = 27$) containing 108 atoms was created.

The simulations were run with the number of particles (N) and pressure (P) remaining constant. Periodic boundary conditions were used in all the simulations. The simulation was conducted at 0 Kelvin and pressure of 0 GPa.

5. RESULTS AND DISCUSSION

The metals and their alloys were simulated using the GULP simulation code 5.1. For each sample the simulation was done first using the MEAM-2NN and then Sutton-Chen inter-atomic potential. The Newton-Raphson optimiser with BFGS hessian updater [1] was used in the optimization process. For optimized structure the elastic constants and bulk and shear moduli were calculated. The results of our computations are presented in Table 2 and on figures 2–3. The the values recorded under the time column in table 2 corresponds to the time taken by the central processing unit (CPU) of the computer to complete the simulation in seconds while the values given under PDM correspond to the peak dynamic memory of the computer used in the simulation process. The experimental values in Table 2 are obtained from different articles in the literature.

The comparison of the CPU computational time taken to complete the simulation for each metal or alloy using the MEAM-2NN and Sutton-Chen potential is shown in figure 2. The time taken by MEAN-2NN is a little less than twice the time taken by the SC potential to complete the task. The value of CPU time by MEAM-2NN falls in the interval $1.79 \times SC_{time} < MEAM - 2NN_{time} < 1.88 \times SC_{time}$. Here SC_{time} refers to CPU time taken when using Sutton-Chen potential in the simulation while $MEAM - 2NN_{time}$ corresponds to the CPU time taken when MEAM-2NN is used in the simulation. Computations using SC potential are fast and this can be attributed to it's simple mathematical formalism.

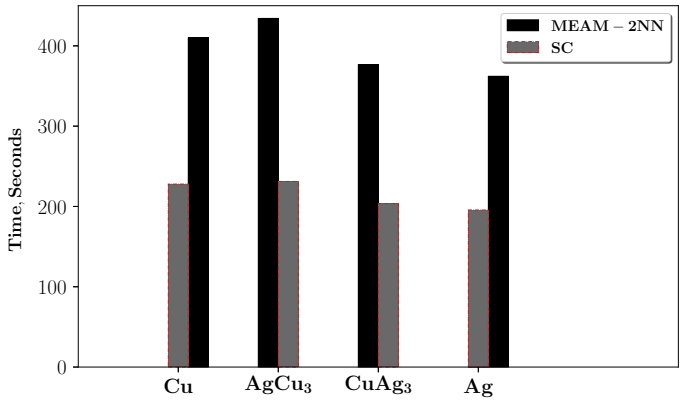

Figure 2. Comparison CPU time in computing Mechanical Properties of the materials using the MEAM-2NN and Sutton-Chen (SC) Potentials.

Table 2. Mechanical properties of the alloy system $Cu - Ag$ using MEAM-2NN and Sutton-Chen (SC) potentials. The Exp. value for each row corresponds to the experimental value. C_{11}, C_{12}, C_{44}, B and G in GPa, time in seconds, peak dynamic memory(PDM) in MB, acoustic velocities(V_t and V_l) in km/s and a in Å.

Metal	Potential	a	C_{11}	C_{12}	C_{44}	B	G	$Time$	PDM	V_t	V_l
Cu	meam-2NN	3.613	176.14	124.91	81.77	141.99	51.44	409.89	8.30	2.40	4.85
	SC	3.611	168.70	129.43	58.17	142.52	37.67	227.88	3.05	2.04	4.64
	Exp.	3.61^a	176.22^b	124.96^b	81.70^b	142.026^a	48^c			2.337^f	4.798^f
$AgCu_3$	meam-2NN	3.750	194.20	129.77	88.59	151.25	59.07	434.17	8.16	2.51	4.95
	SC	3.830	157.70	112.22	60.99	127.38	41.07	231.15	3.22	2.15	4.54
$CuAg_3$	meam-2NN	3.960	155.14	110.40	64.45	125.31	42.20	376.32	7.23	2.02	4.19
	SC	4.1504	121.04	83.18	50.14	95.80	33.94	203.55	3.22	1.94	3.96
Ag	meam-2NN	4.073	131.45	97.31	51.08	108.69	32.95	362.10	7.07	1.76	3.79
	SC	4.280	106.65	72.94	44.88	84.17	30.31	195.63	3.05	1.82	3.69
	Exp.	4.079^e	131.36^b	97.72^b	51.26^b	103.8^d	30^c			1.730^f	3.770^f

^{a} = Ref[15], ^{b} = Ref[23], ^{c} = Ref[24], ^{d} = Ref[25], ^{e} = Ref[26], ^{f} = Ref[27]

The values of the elastic constants C_{11}, C_{12}, C_{44} and the bulk modulus (B) computed using the MEAM-2NN potential for the pure metals Cu and Ag are approximately equal to their respective experimental values where as shear modulus is higher by approximately 3 units.

The value of the elastic constants for Cu computed using the SC potential differ approximately for C_{11} by 8 units, C_{12} by 5 units and C_{44} by 23 units while the value for the bulk modulus is approximately equal to the experimental value. Similarly for Ag, the values are approximately less than the experimental ones for C_{11} and C_{12} by 25 units and for C_{44} by 7 units while the value for the bulk modulus is approximately less than the experimental value by 24 units. The value of the shear modulus is approximately equal to the value from experiment.

The mechanical properties for the alloys were not compared due to lack of experimental data. Generally, the values obtained using the MEAM-2NN are closer to the experimental values when compared for those computed using SC potential. In addition the values of the lattice parameter by both potentials for Cu are approximately equal to the experimental

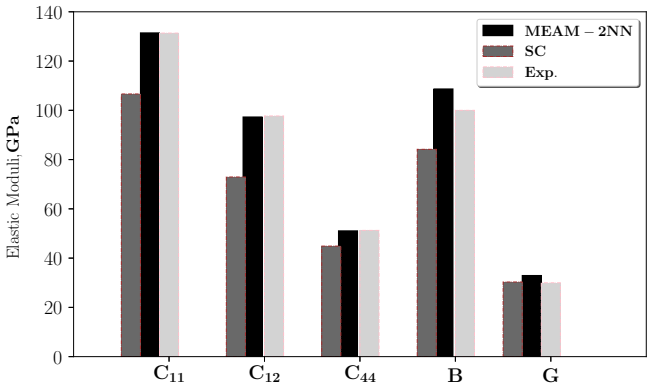

Figure 3. Comparison of the Mechanical Properties of Ag using the MEAM-2NN and Sutton-Chen (SC) Potentials

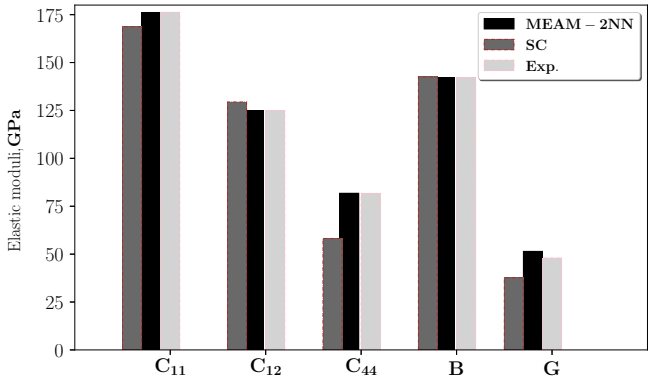

Figure 4. Comparison of the Mechanical Properties of Cu using the MEAM-2NN and Sutton-Chen (SC) Potentials

value. The lattice parameter value for the pure metal Ag by the MEAM-2NN is approximately equal to the experimental value while the result obtained using SC is a little higher than the experimental value.

The peak dynamic computer memory used in the simulation of the alloys system $Cu - Ag$ when the MEAN-2NN interatomic potential used is on average higher by 245% in comparison to the Sutton-Chen model. The acoustic velocities computed using the two models for both metals are close to experimental values. In general terms, the results using MEAM-2NN model are very close to the experimental values while when the SC interatomic potential is used the results are not close to experimental values except for the bulk modulus for Cu and shear modulus for Ag. Generally, the SC method did a poor job in approximating the mechanical properties for Ag in comparison with the MEAM-2NN model.

6. Conclusion

We present a comparative study of mechanical properties of Cu, Ag, $AgCu_3$ and $CuAg_3$ using MEAM-2NN and Sutton-Chen mathematical models. Although these semi-

empirical methods are based on classical laws, the simulation results show that the estimated mechanical properties using the methods are very close to experimental values.

The MEAM-2NN method approximates very well the elastic constants C_{11}, C_{12} and C_{44} for pure metals Cu and Ag. In fact, the results are approximately equal to the experimental values. The same can be concluded about the bulk modulus for the metals Cu and Ag while the value for shear modulus is higher by approximately 3 units from the experimental values. The results obtained using SC potential for the elastic constants and shear modulus are less accurate in comparison with the values obtained using MEAM-2NN. The SC potential approximates very well the bulk modulus for the metal Cu which is approximately equal to the experimental value. The elastic constants and moduli of Ag were poorly approximated by the SC mathematical model. For both pure metals, the MEAM interatomic potential is a significantly better model for approximating transverse and longitudinal acoustic velocities. Hence the MEAM-2NN is a much better model to simulate the mechanical properties of the pure metals Cu and Ag in terms of the closeness the obtained results to the experimental values. The case could be similar with alloys of Cu and Ag but our comparison was hindered due to the lack of experimental data on mechanical properties of the alloys.

The MEAM-2NN model has a substantially greater peak dynamic memory usage than the Sutton-Chen mathematical model. MEAM-2NN simulation is slower than SC potential. MEAM-2NN takes about twice as long as SC potential to run a simulation. The complexity and simplicity of their mathematical formalisms, respectively, could explain the relative speed difference in completing the task of simulation. Furthermore, the MEAM-2NN technique takes into account atoms up to their second closest neighbours. For small metal and alloy systems, the MEAM-2NN model may be superior, however the SC mathematical model may be preferable for complex and larger metal and alloy systems.

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