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Choice of appropriate force field is one of the main concerns of any atomistic simulation that needs to be seriously considered in order to yield reliable results. Since investigations on the mechanical behavior of materials at micro/nanoscale have been becoming much more widespread, it is necessary to determine an adequate potential which accurately models the interaction of the atoms for desired applications. In this framework, reliability of multiple embedded atom method based interatomic potentials for predicting the elastic properties was investigated. Assessments were carried out for different copper, aluminum, and nickel interatomic potentials at room temperature which is considered as the most applicable case. Examined force fields for the three species were taken from online repositories of National Institute of Standards and Technology, as well as the Sandia National Laboratories, the LAMMPS database. Using molecular dynamic simulations, the three independent elastic constants, $C_{11}$, $C_{12}$, and $C_{44}$, were found for Cu, Al, and Ni cubic single crystals. Voigt-Reuss-Hill approximation was then implemented to convert elastic constants of the single crystals into isotropic polycrystalline elastic moduli including bulk modulus, shear modulus, and Young’s modulus as well as Poisson’s ratio. Simulation results from massive molecular dynamic were compared with available experimental data in the literature to justify the robustness of each potential for each species. Eventually, accurate interatomic potentials have been recommended for finding each of the elastic properties of the pure species. Exactitude of the elastic properties was found to be sensitive to the choice of the force fields. Those potentials that were fitted for a specific compound may not necessarily work accurately for all the existing pure species. Tabulated results in this paper might be used as a benchmark to increase assurance of using the interatomic potential that was designated for a problem. Published by AIP Publishing.

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INTRODUCTION

There has been a growing interest in understanding the mechanical properties of nanosized structures, such as nanowires, nanofilms, nanoplates, nanotubes, and nanocrystals, due to their emergence in various areas of science and technology such as nanoelectromechanical systems (NEMS). Investigations regarding the elastic properties of nanocomponents are playing important roles in determining the NEMS sensitivity and the speed of response. Therefore, many experimental, computational, and theoretical studies in this field have been intensively reported in the recent years. Experimentally, Cuenot et al. studied surface tension effect on the mechanical properties of lead nanowires and polypyrrole nanotubes using atomic force microscopy. They found that decreasing the diameter of the nanomaterial led to an increase in the modulus of elasticity. Fonseca et al. proposed a model to predict the elastic properties of the composite material of an amorphous nanowire. They presented experimental setup for two scenarios: (a) static configuration in which the nanowire was maintained twisted and (b) the twisting and tensioning of a nanowire. Peng et al. experimentally studied size-dependent mechanical properties of single crystalline nickel nanowires with different diameters from 100 to 300 nm and crystalline orientations using in-situ tensile tests in a scanning electron microscope. Their important observations were that critically resolved shear stress strongly depended on the sample’s crystalline size and was independent of its orientation. Using the same method, Li et al. obtained mechanical properties of individual InAs nanowires, synthesized by metal organic chemical vapor deposition and molecular beam epitaxy, and determined that Young’s modulus had no dependency on nanowire diameter. Computationally, Liang and Upmanyu studied the size-dependent elasticity of copper nanowires using molecular statics approach based on the embedded atom method (EAM) potential developed by Mishin et al. They concluded that the Young’s modulus of the nanowire was lower than that of bulk copper strained to an equivalent compressive strain. They also found that the nanowire surface was always softer than the (equivalent) bulk. Yuan and Huang investigated the size-dependent elasticity of amorphous silica nanowire using molecular dynamics simulation (MDS). Their results showed that method of sample preparation significantly affected the elastic response of silica nanowires. Moreover, they concluded that overall elasticity could be controlled through the coupling between the surface stiffening and the core softening. Liu et al. used atomistic
simulations to investigate the role of the surface on the size-dependent mechanical properties of copper nanowire with diameters ranging from 2 to 20 nm under tensile load. Their molecular dynamics results verified that the elastic properties of the nanowire were directly associated to the proportion of surface to bulk type atoms. Zanjani and Lukes\textsuperscript{12} investigated the size effect on Young’s modulus, bulk modulus, and Poisson’s ratios of CdSe nanocrystal superlattices using fully atomistic MDS, coarse-grained models, and effective medium theory. They found that the fully atomistic models were the most reliable method because of its good agreement with previously reported results in the literature dealing with a similar system. They also concluded that with increasing nanocrystal core size, Young’s modulus and bulk modulus increased, while it led to a decrease in Poisson’s ratio. Based on a developed modified core-shell model, Hai-Yan et al.\textsuperscript{13} investigated the effect of surface elasticity on Young’s modulus to the bending of nanobeams. They found significant size-dependent effect of elastic modulus with characteristic size reduction, especially below 100 nm. Wang et al.\textsuperscript{14} studied the dependency of Young’s modulus to size and temperature for a silicon nanowire based on a semi-continuum approach. Their results showed that Young’s modulus decreased while temperature increased. They also found that the thickness of nanowire influenced the elastic property of the silicon nanowire with its thickness less than 10 nm and remained constant when it was thicker. Further theoretical, numerical, and experimental investigations regarding mechanical properties of nanostructures can be seen in Refs. 15–18.

Molecular dynamics simulation (MDS) has become a major interest for researchers as a powerful modeling tool in solving various micro/nanoscale problems in number of fields such as biophysics, biochemistry, material science, engineering, and structural biology.\textsuperscript{19–23} Among different potentials that can be applied for MDS, the embedded-atom method (EAM)\textsuperscript{24} is a widely used pair-wise interatomic potential for metallic systems and their alloys. Initial form of EAM potential introduced in Ref. 24 had certain limits in predicting some physical phenomena, and afterward some improvements were made by scientists for different purposes. Therefore, many EAM interatomic potentials for different pure species and their alloys are generated based on different fitting criteria in the literature and most of them can be found in interatomic potentials repository of National Institute of Standards and Technology (NIST)\textsuperscript{25} and the LAMMPS database from Sandia National Laboratories.\textsuperscript{26} However, it is aware that limited works have been done in the recent years to show the significance of implementing an appropriate force field, also known as interatomic potentials, for MDS in conducting an accurate simulation. Suggestions regarding this topic have been released by Becker et al.\textsuperscript{27} via considering the significance of appropriate choice of force field in materials science and engineering through giving some examples and investigation of the elastic constant for aluminum, using some of the Al interatomic potentials managed by the NIST Interatomic Potentials Repository (IPR).

Trautt et al.\textsuperscript{28} discussed the automation of stacking fault energy calculations and their application to additional elements by explaining how the calculations can be modified using the Python script. They compared the fault energy obtained by different interatomic potentials of different elements with the results of the density functional theory. Kalindini et al.\textsuperscript{29} considered the application of data science tools to quantify and to distinguish between structures and models in molecular dynamics datasets. They examined the Al potentials in the IPR to the variation of the principal component scores as a function of temperature for the different force fields. Their results also indicated the utility and the viability of utilizing rigorous structure quantification protocols to the results predicted by MD.

Since each interatomic potential is generally based on a specific problem and fit to reference data within a certain range of composition, temperature, and structure, outside of that range, the interatomic potential may not provide physically meaningful results. In the other words, it is very difficult to develop a universal interatomic potential that works appropriately for all applications. On the other hand, the robustness, accuracy, and validity of an atomistic simulations hinge on the appropriate choice of force fields. Hence, it is necessary to make sure that the performance of an interatomic potential is adequate for a specific purpose with desired condition. To serve this objective and make a shortcut for users to find their best force fields, meanwhile increasing their assurance among so many available interatomic potentials, a number of force fields are examined in this work for the three popular metallic materials Cu, Al, and Ni which are popular in the micro/nano-scale science and technologies. Room temperature which is the most applicable and realistic case to test the materials’ properties is considered in the current simulations. Using molecular dynamic simulation, elastic properties of the cubical single crystals will be computed based on the stress-strain curves by imposing uniaxial tensile as well as shear strains to the system. The predicted elastic constants are compared with experimental values with the purpose of determining which potentials are accurate for the interested metals. Eventually, based on the Voigt-Reuss-Hill (VRH) approximation,\textsuperscript{30} single crystals’ elastic constants are converted into isotropic elastic moduli; thereafter, those values can be meaningfully compared with the experimental values for copper, aluminum, and nickel.

### COMPUTATIONAL DETAILS

Regarding with the materials mechanical properties, this should be noted that the single-crystal elasticity will not be isotropic in general. The number of independent material parameters depends on the level of symmetry of the crystal structure. In fact, the general form of the Hooke’s law for the 36 elastic constants is given by the following stiffness tensor:

\[
C = \begin{bmatrix}
C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\
C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\
C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\
C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\
C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\
C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66}
\end{bmatrix}.
\]
For the cubic structure, the elasticity matrix can be written in terms of three independent elastic stiffness constants since \( C_{11} = C_{22} = C_{33}, C_{12} = C_{23} = C_{32} = C_{13} = C_{31}, \) and \( C_{44} = C_{55} = C_{66} \) because \( x-, y-, \) and \( z- \) axes are identical by symmetry. In addition, the off diagonal shear components are zero which means \( C_{45} = C_{46} = C_{54} = C_{56} = C_{64} = C_{65} = C_{96} = 0. \) So the stiffness tensor can be simplified into a three variable independent form as

\[
C = \begin{bmatrix}
C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{44}
\end{bmatrix} \tag{2}
\]

So, for a cubic single crystal, three independent elastic constants, \( C_{11}, C_{12}, \) and \( C_{44} \) are going to be found using each interatomic potential.

Elastic constants \( C \) relate the strain \( \varepsilon \) and the stress \( \sigma \) in a linear fashion:

\[
\sigma_{ij} = \sum_{kl} C_{ijkl} \varepsilon_{kl} \tag{3}
\]

which relates to elastic energy density \( U \) that is defined as follows\textsuperscript{33} for a cubic crystal \( x \)-along \([100], y \parallel [010], \text{and } z \parallel [001] \)

\[
U = \frac{1}{2} C_{11} \left( \varepsilon_{xx}^2 + \varepsilon_{yy}^2 + \varepsilon_{zz}^2 \right) + \frac{1}{2} C_{44} \left( \varepsilon_{xy}^2 + \varepsilon_{xz}^2 + \varepsilon_{yz}^2 \right) \\
+ C_{12} (\varepsilon_{yx} \varepsilon_{zz} + \varepsilon_{yz} \varepsilon_{xx} + \varepsilon_{xz} \varepsilon_{yy}), \tag{4}
\]

where \( \varepsilon_{ij} \) are strain components by the relations:

\[
\begin{align*}
\varepsilon_{xx} & \equiv \frac{\partial u}{\partial x}; & \varepsilon_{yy} & \equiv \frac{\partial v}{\partial y} = \frac{\partial v}{\partial x} & \varepsilon_{zz} & \equiv \frac{\partial w}{\partial z}; \\
\varepsilon_{xy} & \equiv \varepsilon_{yx} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}, & \varepsilon_{xz} & \equiv \varepsilon_{zx} = \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}, & \varepsilon_{yz} & \equiv \varepsilon_{zy} = \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y};
\end{align*}
\]

where \( u, v, \text{ and } w \) are displacements in \( x-, y-, \text{ and } z- \) directions, respectively.

Further, from (4),

\[
\frac{\partial U}{\partial \varepsilon_{ij}} = \sigma_{ij}. \tag{6}
\]

Therefore, we derive the followings according to (3) or (6)

\[
\sigma_{xx} = C_{11} \varepsilon_{xx} + C_{12} (\varepsilon_{xy} + \varepsilon_{xz}), \tag{7}
\]

\[
\sigma_{yy} = C_{11} \varepsilon_{yy} + C_{12} (\varepsilon_{xx} + \varepsilon_{xz}), \tag{8}
\]

\[
\sigma_{zz} = C_{11} \varepsilon_{zz} + C_{12} (\varepsilon_{xx} + \varepsilon_{xy}), \tag{9}
\]

\[
\sigma_{xy} = C_{44} \varepsilon_{xy} + C_{44} \varepsilon_{yx} = C_{44} \varepsilon_{xy}, \tag{10}
\]

where \( \varepsilon_{xy} \) is also known as \( \gamma_{xy} \), which is the engineering shear strain.

On the simulations to find the three independent elastic constants, large-scale atomic/molecular massively parallel simulator (LAMMPS), a classical molecular dynamics solver, is used for the current work.\textsuperscript{34} A cubic box with size of \( 70a \times 70a \times 70a \) is created for copper, aluminum, and nickel with lattice constant \( a \). The periodic boundary condition is applied in the \( x-, y-, \) and \( z- \) directions to find the bulk properties for comparison with experimental data in the literature. The materials being considered are pure substance of solid \( Cu, Al, \) and \( Ni \) arranged in the face centered cubic (FCC) fashion. Different styles of the EAM potential are adopted in the simulations. According to Daw and Baskes,\textsuperscript{24} the potential energy of an embedded atom \( i \) can be approximated as

\[
E_{int} = \sum_i F_i (\rho_{h,i}) + \frac{1}{2} \sum_{i,j \neq i} \phi_{ij}(R_{ij}), \tag{11}
\]

where \( F_i (\rho) \) is the embedding energy for embedding atom \( i \) into the host electron density \( \rho \), and \( \phi_{ij}(R_{ij}) \) is the pair potential which is a function of the distance \( R \) between atoms \( i \) and \( j \). The \( \rho_{h,i} \) represents the host electron density at atom \( i \) due to the remaining atoms of the system which is approximated by the superposition of atomic densities as follows:

\[
\rho_{h,i} = \sum_{j \neq i} \rho_i^a(R_{ij}), \tag{12}
\]

where \( \rho_i^a(R) \) is the electron density at the site of atom \( i \) due to the presence of atom \( j \) at a distance of \( R \).

The potential functions in (11) and (12) are usually treated as some fitting functions which are proposed by some researchers in consideration of the physical properties of the interested metals as well as their alloys. Generally, the EAM potential is simple; however, its embedded energy and pair potential are given in the form of spline functions which leads to some inconvenience for calculations.\textsuperscript{35} This explains why there are so many EAM based interatomic potentials developed or optimized in the literature. In this paper, the fitted functions of EAM based potentials generated for a specific compound or a pure species are examined to obtain elastic constants of a cubic single crystal and different elastic moduli for the three elements. To achieve this, the single crystal \( Cu, Al, \) and \( Ni \) lattices need to be deformed under a uniaxial and a shear strain, independently.

Finding elastic constants at finite temperature is a little tricky and more complicated with respect to zero-temperature properties. That is why users need to pay more attention to the system equilibration, constrains, and methods of calculations. Here, the simulation procedure for finding the three independent elastic constants of cubical single crystals is explained in detail.

First, an instantaneous temperature of 500 K was defined in terms of the instantaneous kinetic energy to generate an ensemble of velocities using a random number generator with the specified seed as the specified temperature. Then, the entire system was equilibrated at temperature of 500K using NVT dynamics, for 10 ps. Time step \( \Delta t = 1fs \) is used throughout the simulations. After that, the relaxation was continued with the same temperature for 25 ps using isothermal-isobaric (NPT) ensemble. In the next stage of relaxation, the structure
was cooled down to the desired temperature of 300 K for 25 ps followed by a duration of 25 ps at the same temperature. It is worth to note that, in all equilibration stages, linear momentum was zeroed by subtracting the center-of-mass velocity of the group from each atom. To calculate the anisotropic elastic stiffness constants, $C_{11}$ and $C_{12}$, a simple uniaxial tensile strain rate of $10^{-3}$ ps$^{-1}$ (strain increases 0.1% every picosecond) was applied along the [100] (x-direction) at 300 K which leads to nonzero stress components $\sigma_{xx}$, $\sigma_{yy}$, $\sigma_{zz}$. The strains in the y- and z-directions were both controlled to be zero under the NVT ensemble to find the two stiffness constants based on (7) and (8) having $\varepsilon_{yy} = \varepsilon_{zz} = 0$. Once the stress-strain curves are obtained, it is straightforward to find the $C_{11}$ and $C_{12}$ from the slope of the linear part of $\sigma_{xx}$ and $\sigma_{yy}$ versus strain, respectively. Figure 1 displays a schematic of the two created atomistic systems under the applied uniaxial tensile and shear strains.

To find $C_{44}$, a prism region was created rather than a block that was used for the uniaxial strain, to define a triclinic simulation box with initial tilt factors of zero. Then, with the same equilibration steps and under the NVT ensemble, the system was distorted in the [110] direction by applying an engineering shear strain rate of $10^{-3}$ ps$^{-1}$ so that the crystal is no longer cuboidal. Afterward, $C_{44}$ has been calculated by finding the slope of linear portion of yield curve for $\sigma_{xy}$ versus the associated strain $\varepsilon_{xy}$ according to (10).

Once the elastic constants using different potentials are found, using the Voigt-Reuss-Hill approximation, which is an averaging scheme, the anisotropic single-crystal elastic constants can be converted into isotropic polycrystalline elastic moduli. For a single-phase crystalline aggregate made of crystals that are slightly anisotropic, the approximation gives the realistic values of isotropic elastic moduli. This approach combines the upper and lower bounds by assuming the average of values obtained through the Voigt and Reuss averaging methods. In the upper bound (Voigt), the strain assumes to be uniform and continuous, whereas the stresses are allowed to be discontinuous. In the lower bound (Reuss), the stresses are assumed to be continuous and the strains can be discontinuous.

Bulk modulus is defined as follows:

$$B = \frac{C_{11} + 2C_{12}}{3},$$  \hspace{1cm} (13)

and the upper and lower bounds of shear moduli are

$$G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5},$$  \hspace{1cm} (14)

and

$$G_R = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})},$$  \hspace{1cm} (15)

based on the Hill empirical average, we have the isotropic elastic shear modulus as follows:

$$G_{VRH} = \frac{G_V + G_R}{2}. \hspace{1cm} (16)$$

Knowing shear modulus $G$ and bulk modulus $B$, it is then straightforward to find Young’s modulus $E$ and Poisson’s ratio $\nu$ from the well-known isotropic relations as follows:

$$E = \frac{9GB}{3B + G},$$  \hspace{1cm} (17)

and

$$\nu = \frac{3B - 2G}{2(3B + G)}. \hspace{1cm} (18)$$

RESULTS AND DISCUSSION

Results, using different classes of potentials, eam, eam/alloy, and Finnis-Sinclair, for three independents elastic stiffness constants of Cu, Al, and Ni single crystals are tabulated in Tables I–III. Elastic constants $C_{11}$, $C_{12}$, and $C_{44}$ were found from the slope of the elastic regime of the stress-strain curves, where the growth of stress versus strain is linear. These elastic stiffness constants were obtained

FIG. 1. Schematic of applied uniaxial and shear strains to the atomistic systems.
using a curve fitting technique by defining a stipulation that in linear regression, the $R^2$ coefficient of determination should be greater than 0.999 to achieve an accurate judgment on the results as much as possible. This is the reason that a large simulation box with more than a million atoms was created to minimize the temperature deviation due to thermal velocity fluctuations and thereafter yield a smooth linear stress versus strain relation rather than an oscillatory one. Figure 2 shows the effect of number of atoms on simulation temperature through the applied strains. As can be seen, increasing the number of atoms decreases the deviations from desired temperature which leads to a more smooth line for stress-strain curve and eventually a better and more reliable linear fit. Furthermore, it is obvious from Fig. 2 that deviation from 300 K is about 40 K for 500\textsuperscript{1/2}10\textsuperscript{6} atoms, which completely makes sense from statistical mechanics point of view.

<table>
<thead>
<tr>
<th>Copper potentials</th>
<th>$C_{11}$</th>
<th>Error (%)</th>
<th>$C_{12}$</th>
<th>Error (%)</th>
<th>$C_{44}$</th>
<th>Error (%)</th>
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<th>$C_{12}$</th>
<th>Error (%)</th>
<th>$C_{44}$</th>
<th>Error (%)</th>
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Simulation results based on each interatomic potential have been compared with experimental data available in the literature at temperature of 300 K, and meanwhile, the corresponding relative errors are reported. It should be noted that one may find less/more relative errors with respect to experimental values by using a different criterion, such as using R-squared value less than 0.999.

As seen in Tables I–III, most of the examined potentials are yielding acceptable results in predicting all the three elastic constants according to their relative errors. Tables I–III also exemplify that some of the interatomic potentials are capable for accurate determination of one or two elastic constant rather than all, and may fail for the other one(s). This is the reason that user must be very careful about whether the force field works well for their interested problem or not. As an example in Table II, Mishin-Ni-Al-Co-2013.eam.alloy predicts the $C_{11}$ and $C_{12}$ for the aluminum with relative errors less than 1% while yield 16.18% and 17.31% error for $C_{44}$, respectively. On the contrary, Ni1_Mendelev_2012.eam.fs predicts nickel $C_{11}$ and $C_{12}$ with about 20.00% error while yields the $C_{44}$ with 3.42% error. In another scenario, a potential like Ni_u6.eam gives 4.30% and 0.99% error for $C_{12}$ and $C_{44}$, respectively, but predicts $C_{11}$ with 18.45% error from experimental result.

Furthermore, among the potentials that have been created for a specific compound, they may work well for one or some of the elements but poorly predict the elastic properties for the others. For instance, FeCuNi.eam.alloy predicts the $C_{11}$ and $C_{12}$ with about 20.00% error while yields the $C_{44}$ with 3.42% error. In another scenario, a potential like Ni_u6.eam gives 4.30% and 0.99% error for $C_{12}$ and $C_{44}$, respectively, but predicts $C_{11}$ with 18.45% error from experimental result. Furthermore, among the potentials that have been created for a specific compound, they may work well for one or some of the elements but poorly predict the elastic properties for the others. For instance, FeCuNi.eam.alloy predicts the $C_{11}$ and $C_{12}$ with about 20.00% error while yields the $C_{44}$ with 3.42% error. In another scenario, a potential like Ni_u6.eam gives 4.30% and 0.99% error for $C_{12}$ and $C_{44}$, respectively, but predicts $C_{11}$ with 18.45% error from experimental result.

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Afterward, single crystal elastic stiffness constants have been converted into isotropic elastic moduli including bulk modulus, shear modulus, and Young’s modulus as well as Poisson’s ratio in Figures 3–14 using VRH approximation for different interatomic potentials listed in Tables I–III. Simulation results are compared with the experimental ones for Cu,$^{44,45}$ Al,$^{36,47}$ and Ni$^{48,49}$ for these interesting mechanical properties.

<table>
<thead>
<tr>
<th>Nickel potentials</th>
<th>$C_{11}$ Error (%)</th>
<th>$C_{12}$ Error (%)</th>
<th>$C_{44}$ Error (%)</th>
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<td>Ni-Zr_Mendelev_2014.eam.fs$^{79}$</td>
<td>206.32</td>
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<td>Ni1_Mendelev_2012.eam.fs$^{80}$</td>
<td>206.73</td>
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FIG. 2. (a) Effect of number of atoms on deviation of temperature from desired one. (b) Uniform temperature near to 300 K with more than one million atoms.
Figures 3–5 show the bulk modulus of the three studied species obtained by each elemental potential and present the deviation of MDS results from experimental data. According to Fig. 3, among examined elemental potentials, copper bulk modulus can be accurately obtained using Cu-Zr._eam.fs, Cu-Zr.eam.fs, Cu1.eam.fs, and Mendelev Cu2_2012.eam.fs with less than 3.00% relative error from experimental value and also FeCuNi.eam.alloy, Cu_mishin1.eam.alloy, CuAg.eam.alloy, and Cu01.eam.alloy with less than 4.50%. As can be seen from (13), bulk modulus depends only on the two independent elastic constants $C_{11}$ and $C_{12}$. It is found from Fig. 3 that potentials successfully predicted these two elastic constants show their capability in predicting bulk modulus accurately as well. However, on the other hand, a question arises according to Fig. 4.

FIG. 3. Copper bulk modulus predicted by different force fields.

FIG. 4. Aluminum bulk modulus predicted by different force fields.
4 that why some potentials fail to predict both $C_{11}$ and $C_{12}$ accurately, but they succeed in predicting bulk modulus? How logical and reliable they are? The answer to this question is that, while bulk modulus is the result of an algebraic expression, two inaccurate variables can also lead to a desirable value. It is absolutely fortuitous and unreliable potential to account on that for users’ simulation in considering the present problem. Sensible instances of this kind of deceptive observations for bulk modulus results are $Al_{jnp}.eam$ and $AlO.eam.alloy$ for aluminum according to Fig. 4 and Table II. This can spark

![Graph 1](image1.png)

**FIG. 5.** Nickel bulk modulus predicted by different force fields.

![Graph 2](image2.png)

**FIG. 6.** Copper shear modulus predicted by VRH approximation using different force fields.
a debate on the way of finding bulk modulus. So, this can be concluded that the potentials: Mishin-Ni-Al-Co-2013.eam.alloy, Al99.eam.alloy, Mishin-NiAl2009, Mishin-Al-Co-2013.eam.alloy, Mg-Al-set.eam.alloy, Al-Mg.eam.fs, AlPb-setfl.eam.alloy, Almm, and Al1.eam.fs might be suggested to the users for finding aluminum bulk modulus as they predicted this property with less than 2.00% relative error, and also the two related elastic stiffness constants $C_{11}$ and $C_{12}$ are very close.
to the experimental results with the lowest relative errors. Although it does not mean that other potentials are not effective or applicable, users according to their problem and demand may use the other ones which are yielding acceptable errors. Therefore, one may read the original reference of each potential and see for what purpose it has been developed, and according to what reference data they were fitted. To confirm this statement, continuously readers will see that other potentials may be recommended for finding the other elastic properties rather than or further to what mentioned above for each species.

According to Fig. 5, for nickel, the two FeNiCr_Bonny_2013_ptDef.eam.alloy and Ni.eam.fs predict the nickel bulk Young's modulus.
modulus with 2.42% and 1.95% relative errors with respect to experimental values, respectively. However, most of the examined potentials for nickel may predict an acceptable value with a relative error around 11% such as Ni_u3.eam, Ni_u6.eam, Mishin-Ni-Al-Co-2013.eam.alloy, Ni_smf7.eam, Fe-Ni.eam.alloy, CuNi.eam.alloy, Mishin-Ni-Co-2013.eam.alloy, NiAl.eam.alloy, Mishin-Ni-Al-2009.eam.alloy, FeCuNi.eam.alloy, and Ni99.eam.alloy, but they may not be as...
powerful as the two mentioned ones in predicting both of the stiffness constants. Figure 5 also confirms this postulate that some of the interatomic potentials which have been created for a compound or alloy system do not necessarily work well for all the existing elements. The two good examples for this statement are Mishin-Ni-Al-Co-2013.eam.alloy and Mishin-Ni-Al-2009.eam.alloy that are very accurate for Al bulk modulus with less than 2.00%, while they are not this much accurate for Ni and also its elastic stiffness constants. FeCuNi.eam.alloy is another one which is much more accurate for Cu than Ni.

These elastic moduli for the three elements are displayed in terms of VRH approximation with the Voigt and Reuss bounds shown in Figures 6–14. Figures 6–8 depict the shear modulus obtained for the three species based on elastic stiffness constants via different potentials. According to Fig. 6, the accurate copper potentials introduced for bulk modulus are accurate for finding shear modulus though. The difference is increasing their error from experimental result up to 3%–4%. The reason is that, for calculating shear modulus, Young's modulus, and Poisson's ratio of an isotropic polycrystalline, in addition to $C_{11}$ and $C_{12}$, $C_{44}$ plays an important role in predicting these elastic properties. This fact has a significant effect on choice of appropriate potential for predicting shear modulus further to/rather than those recommended for finding bulk moduli since $C_1$ potentials are found to be more precise in finding $C_{11}$ and $C_{12}$ compared with $C_{44}$ according to Table I. In this regard, the role of the other potentials that can predict shear moduli more accurately with an acceptable error for the three elastic constants comes in. For aluminum, it can be obtained from Fig. 7 that NiAl.eam.alloy, Al-Mg.eam.fs, Zope-

![FIG. 13. Aluminum Poisson's ratio predicted by VRH approximation using different force fields.](image-url)
expression and make the scenario much more complicated. Therefore, it is highly recommended that users pay attention to the accuracy of the elastic constants which are also able to estimate accurate isotropic elastic moduli.

CONCLUSION

Adequate choice of interatomic potential, as a frequent concern in conversations among the molecular dynamic simulation community, was studied for finding the three independent elastic stiffness constants, the $C_{11}$, $C_{12}$, and $C_{44}$, of copper, aluminum, and nickel cubic single crystals. The three independent stiffness constants of cubic single crystals originated from implementation of all the studied potentials, provided from NIST IPR and LAMMPS database, were determined using a linear regression analysis of the linear part of stress-strain curves. Once elastic constants were obtained, they have been converted into isotropic elastic moduli using Voigt-Reuss-Hill approximation. Bulk modulus, shear modulus, Young’s modulus, and Poisson’s ratio were calculated, and results from each interatomic potential have been compared to the experimental ones both for anisotropic elastic stiffness constants and the converted isotropic elastic modulus. It is concluded that inadequate choice of force field strongly affects the simulation results and gives rise to some inconveniences for calculations. Some of the interatomic potentials seem to be useful and accurate for predicting one or two of the elastic constants or elastic modulus, not all of them. It is also found that the elemental potentials that have been generated for a specific alloy or compound are not expected to necessarily work for all of the present species in the compound. Results presented in this work are useful for interested researchers in the field of atomistic study of materials mechanical properties and increase the assurance of the users to see which interatomic potential fits well to their specific problem.

ACKNOWLEDGMENTS

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