UDC 539.32

NUMERICAL INVESTIGATION OF INFLUENCE OF CHEMICAL DISORDER TO MECHANICAL PROPERTIES OF CU-AG AND AU-AG ALLOYS

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Summary: This work presents simulation results of Cu-Ag and Au-Ag alloy systems. The Sutton-Chen inter-atomic potential was used to model the energy of interaction among the atoms forming the metals and their alloys. For the alloys ordered and chemically disordered configurations were prepared and simulated using gulp. Bulk and shear moduli and elastic constants of the materials were estimated from the simulation. The values of Young's modulus, Pugh's and Poisson's ratios were calculated. The influence of chemical disorder to the mechanical properties of alloys was investigated. The results of the computation were compared with experimental data and research works from different references whenever there is data available for comparison. The results of our calculation show that chemical disorder has significant influence on some of the mechanical properties of alloys while in others it is insignificant.

Keywords: computer simulation; chemical disorder; empirical formulas; interatomic potentials; mechanical properties; ductility.

1 Introduction

The study of material physics with chemical and structural disorder has developed for many decades. The main interest in these investigations is to take into account atomic and electronic structures of the materials. However, the influence of chemical and structural disorder to mechanical properties of alloys is insufficiently studied because in mechanics of deformable solids continuum model is used. Recently, a new scientific approach known as "nanomechanics" is intensively developing. In frame of nanomechanics, materials are studied from their discrete structures. That is in nanomechanics we can investigate the properties of solids by taking into account their atomic structures via the method of molecular dynamics (MD) [1, 2] and other methods.

In our paper we studied the influence of chemical disorder to mechanical properties of alloys such as bulk, shear and Young's moduli and Pugh's and Poisson's ra-

tios. There are many papers devoted to numerical simulations of mechanical properties of ordered alloys ones via first principle calculations and other times via semi-empirical approximations. For example authors of paper [3] studied elastic and thermodynamic properties and structural stability of Au-Cu alloys from first-principles calculations. We used Sutton-Chen semi-empirical models for calculation of mechanical properties of Cu-Ag and Au-Ag alloys.

Metallic alloys are used in industries, power plants, aircraft engines and structural materials [4, 5]. Cu-based alloys find use in many areas of material science applications [6] like electrical components, door handles, coins, jewelry, etc. Silver and gold nanoparticles are used in medical imaging and nanosurgery [7].

The mechanical properties of metals are used to specify the identity and the range of usefulness of the metal. The prediction of mechanical properties of materials before manufacturing them saves money and it could furthermore contribute to the development of supper materials [8]. There is a need for producing noble alloys having specific mechanical and thermodynamic properties. This can be done most effectively by studying the material properties at the nanoscale level. Computer simulation is a powerful technique used to study properties of materials with good accuracy and in a cost effective way [9].

2 Physical Model

Elastic constants, bulk modulus, shear modulus, Poisson's ratio, Young's modulus are important material parameters. These mechanical properties of alloys can be investigated by applying numerical simulation techniques. In our work, all the simulations were performed using General Utility Lattice Program (GULP) code 5.1 [10] which is a free software for academic purposes (http://gulp.curtin.edu.au/gulp/). This molecular dynamics simulation code allows us to make wide-range material property calculations using different inter-atomic potentials [11, 12].

We use Sutton-Chen(SC) model of inter-atomic interaction potential. This physical model is widely used for molecular dynamic simulation of metals and their alloys [4, 13, 14]. It is a semi-empirical interaction potential given as the sum of a pairwise repulsion term and a many-body density-dependent cohesion term [15] and it's mathematical formulation is [16, 17]:

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

where ϵ; c; m and n are parameters optimized by fitting to elastic constants, bulk

modulus and cohesive energy from experiments and r_{ij} is the separation distance between the atoms *i* and *j*. ϵ is measured in electron volt (*e*V), *m* and *n* are integers and *c* is dimensionless quantity. The first term is the core repulsion potential and the second term is bonding energy mediated by the electrons [18].

Table 1 – Sutton-Chen potential parameters for the Cu , Au and Ag metals [19, 20]

Metal	n	m	ϵ (eV)	c	a ($\overset{0}{A}$)
Cu	6	9	1.2382×10^{-2}	39.432	3.6100
Au	8	10	1.2793×10^{-2}	34.408	4.0800
Ag	6	12	2.5415×10^{-3}	144.41	4.0900

Table 1 gives the value of Sutton-Chen parameters for pure metals of Cu, Au and Ag. The parameters for the Cu-Ag and Au-Ag alloys can be estimated using the mixing rules given in [16]. To model the influence of chemical disorder on mechanical properties of alloys: $AgCu_3$ ((25 %) silver and 75 % copper), $CuAg_3$ (25 % copper and 75 % silver), $AgAu_3$ ((25 %) silver and 75 % gold) and $AgAu_3$ ((25 %) silver and 75 % gold) were considered in addition to the pure metals *Cu*, *Au* and *Ag*. The structure of pure metals Cu, Au and Ag is FCC [17].

For each alloy type ordered and chemically disordered configurations were prepared and simulated. For instance, an ordered cubic unit cell of $AgCu_3$ consists of 3 copper atoms and 1 silver atom located in space. It's unit cell was constructed as follows: Ag: *a*(0; 0; 0); Cu: *a*(1/2; 1/2; 0); Cu: *a*(0; 1/2; 1/2); Cu: *a*(1/2; 0; 1/2), where *a* is the edge of an elementary cube. From the unit cell of $AgCu_3$ a supercell of $AgCu_3$ containing 27 elementary cells (3 × 3 × 3) with a total of 108 atoms was constructed. The supercell for the other types of ordered alloys were constructed in similar manner where the element with one atom takes the origin and the remaining three atoms taking the face centers of the elementary cube.

In the chemically disordered alloys, the atoms were arranged in each of the four possible positions in each primary cell using python random program designed for this purpose. Care has been taken so that stoichiometric ratio in each elementary cell was not violated. For example, in each disordered elementary cell of $AgCu_3$, there are one atom of silver and three atoms of copper. In general terms, the elementary cells that compose the disordered supercell are not equivalent to each other.

2.1 Calculation of Bulk Properties

After determining the optimized structure of a pure metal and it's alloy, we can calculated the mechanical properties of the materials [11]. GULP has the facilities to calculate mechanical properties, such as the bulk and shear moduli and elastic constants.

2.2 Elastic Constants

The knowledge of elastic constants of a solid provides access to the understanding of it's mechanical properties for materials [21]. Elastic constants can provide information on the stability, stiffness, brittleness, ductility, and anisotropy of a material [22–24]. They are essential parameters that correlate the microscopic properties to macroscopic mechanical properties. Precise calculation of the elastic constants is essential for gaining insight into the mechanical strength of solids, verifying their stability, and designing material applications [3].

For a general 3-D materials 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 [25]:

$$\sigma_i = C_{ij}\varepsilon_i, \tag{2}$$

where C is elastic constant, σ is stress and ϵ is strain. The stress-strain relation having 36 independent components has a concise matrix form:

$$\begin{pmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\\ \sigma_4\\ \sigma_5\\ \sigma_6\end{pmatrix} = \begin{pmatrix}C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16}\\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26}\\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36}\\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46}\\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56}\\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66}\end{pmatrix}\begin{pmatrix}\varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\\ \varepsilon_4\\ \varepsilon_5\\ \varepsilon_6\end{pmatrix}. \tag{3}$$

GULP has the computational resources for evaluating elastic constants. The potential energy is a functions of atomic coordinates. The second derivative of potential energy function with respect to strain gives elastic constants [11]:

$$C_{ij} = \frac{1}{V}\frac{\partial^2 U}{\partial\varepsilon_i \partial\varepsilon_j}, \tag{4}$$

where U is the total energy expression, C_{ij} represents components of the stiffness matrix C, V is the volume of unit cell under consideration, ϵ_i and ϵ_j are strain. The derivatives of the potential energy function are computed using finite difference methods.

The elastic constants describe the mechanical hardness of the material with respect to deformation. Using the symmetry in a cubic system, the only three independent coefficients are C_{11}, C_{12} and C_{44} which describe the hardness of a given material. Mechanical stability (structural stiffness) of a material determines how much a material deforms under applied load. For the cubic crystal, the mechanical stability criteria is [24]:

$$C_{11} - C_{12} > 0, \qquad C_{11} > 0, \qquad C_{11} + 2C_{12} > 0. \tag{5}$$

2.3 Bulk and Shear Moduli

The bulk modulus is defined as the ratio of the infinitesimal pressure increase to the resulting relative decrease of the volume. The bulk (B) and shear (G) moduli are also related to the hardness of a material with respect to various types of deformations [26].

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) [3, 27]. Hill showed that the Voigt approximation leads to overestimated values of the elastic moduli, while the Reuss approximation underestimated the values [27], and recommended to take the arithmetic mean of value of these approximations [28-30].

The formulas for bulk and shear moduli due to Reuss and Voigt are given below [3, 11]:

$$B_V = \frac{1}{9}\left(C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})\right);$$

$$B_R = \frac{1}{9}\left(S_{11} + S_{22} + S_{33} + 2(S_{12} + S_{13} + S_{23})\right)^{-1};$$

$$G_V = \frac{1}{15}\left(C_{11} + C_{22} + C_{33} + 3(C_{44} + C_{55} + C_{66}) - C_{12} - C_{13} - C_{23}\right);$$

$$G_R = \frac{15}{4\left(S_{11} + S_{22} + S_{33} - S_{12} - S_{13} - S_{23}\right) + 3(S_{44} + S_{55} + S_{66})}.$$

The bulk modulus in the Hill approximation is given as follows [29]:

$$B_H = \frac{B_V + B_R}{2}. \tag{6}$$

For cubic crystals $B_H = B_R = B_V$. The shear modulus G_H in the Hill approximation is calculated in similar manner to the bulk modulus and is presented in the relation below [3]:

$$G_H = \frac{G_V + G_R}{2}, \tag{7}$$

where G_R is the shear modulus in the Reuss approximation and G_V is the shear modulus in the Voigt approximation.

For cubic crystals G_R and G_V can be calculated from elastic constants as follows [28]:

$$G_R = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})}; \tag{8}$$

$$G_V = \frac{3C_{44} + C_{11} - C_{12}}{5}. \tag{9}$$

Ductility is a mechanical property of a material closed related to shear and bulk moduli. Ductility may be described as the ability of a metal to deform without breaking. The ratio $K = B/G$ proposed by Pugh [31] indicates the malleability of the metal. K measures the extent of brittleness or ductility of a given material. If $K < 1.75$ then, the material will behave in brittle manner else it is considered to have a good ductility [32, 33].

2.4 Young's Modulus and Poisson's ratio

Young's modulus, E, is a measure of the ability of a material to withstand changes in length when it is under uni-axial compression. The Young's modulus can be calculated using the relation given below [33, 34]:

$$E = \frac{9BG_H}{3B + G_H}. \tag{10}$$

Young's modulus is vital for different applications. Large value of E indicates the material is stiff. The Poisson's ratio ν defined as the ratio of transverse strain to the longitudinal strain is used to reflect the stability of the material against shear and provides information about the nature of the bonding forces [22]. The Poisson's ratio, ν, can be computed as follows from the values of bulk and shear moduli [33, 35]:

$$\nu = \frac{3B - 2G_H}{2(3B - G_H)}. \tag{11}$$

3 The Calculation Details, Results, and Discussion

Table 2 – Elastic constants C_{11}; C_{12}; C_{44}

Phase	a ($\overset{0}{A}$)	C_{11}(GPa)	C_{12}(GPa)	C_{44}(GPa)
Cu Ref.[3] Exp. from [17]	3.611 3.63 3.61	168.70 177.0 176.20	129.445 118.8 124.94	58.17 82.4 81.8
Au Ref.[3] Exp. from [17]	4.080 4.186 4.078	179.873 147.8 201.6	147.791 143.5 169.7	42:135 38.7 45.4
$AgCu_3$ (ordered)	3.830	157.698	112.221	60.989
$AgCu_3$ (disordered)	3.897	128.875	112.641	31.163
$CuAg_3$ (ordered)	4.150	121.039	83.180	50.142
$CuAg_3$ (disordered)	4.202	102.019	81.1362	42.570
Ag	4.280	106.646	72.939	44.881
$AgAu_3$ (ordered)	4.064	180.938	140.084	47.544
$AgAu_3$ (disordered)	4.070	161.660	132.146	44.713
$AuAg_3$ (ordered)	4.158	143.703	99.865	50.753
$AuAg_3$ (disordered)	4.321	56.576	39.927	32.336

Table 3 – Bulk modulus *B*, shear modulus *G*, Young's modulus *E* (GPa); *K* and ν are dimensionless quantities. Ordered Cu-Ag alloys

Phase	B	G	E	ν	K
$AgCu_3$	127.380	41.073	111.261	0.35	3.101
$CuAg_3$	95.799	33.936	91.055	0.34	2.822
Ag	84.174	30.311	81.188	0.34	2.777

Table 4 – Bulk modulus *B*, shear modulus *G*, Young's modulus *E* (GPa); *K* and ν are dimensionless quantities. Disordered Cu-Ag alloys

Phase	B	G	E	ν	K
$AgCu_3$	119.099	15.025	43.257	0.44	7.926
$CuAg_3$	90.958	20.996	58.489	0.39	4.332

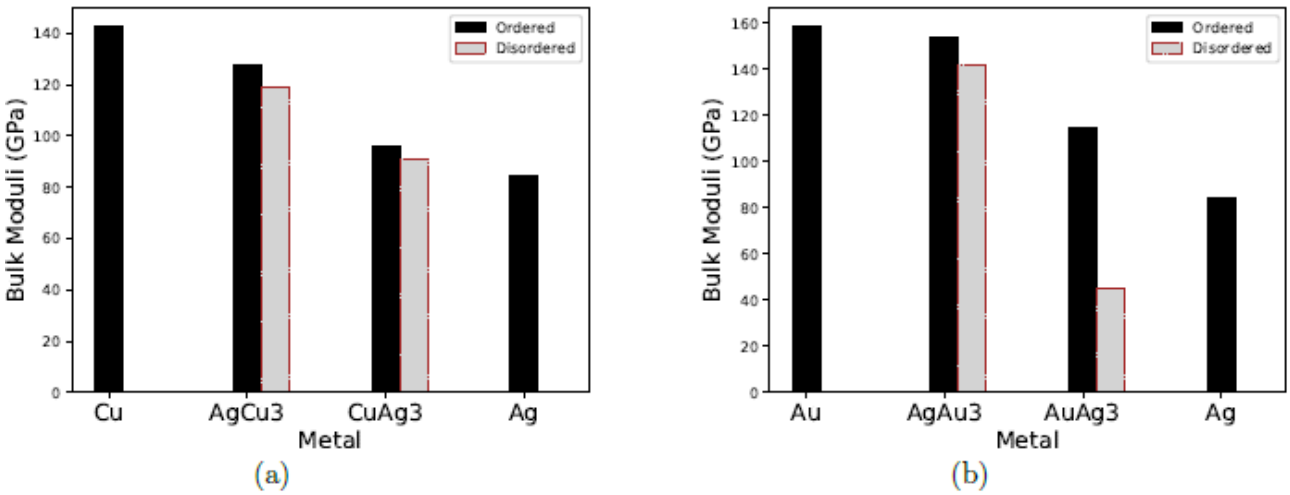

Figure 1 – Comparison of bulk modulus of ordered and disordered alloys: a) Cu-Ag; b) Au-Ag

For each alloy type ordered and disordered configurations were prepared and simulated in GULP under constant pressure and temperature T = 0 Kelvin. The simulation code first optimizes the given structure using energy minimization techniques and then calculates the different mechanical properties for the optimized structure for all the given input files. During the simulation process, the structures for all the ordered alloys optimization was achieved. The optimized structure for the disordered alloys of $AgCu_3$, $CuAg_3$, $AgAu_3$ was obtained while the structure for disordered $AuAg_3$ could not be optimized.

Table 5 – Bulk modulus B, shear modulus G, Young's modulus E (GPa); K and ν are dimensionless quantities. Ordered Au-Ag alloys

Phase	B	G	E	ν	K
$AgAu_3$	153.702	33.875	94.671	0.40	4.537
$AuAg_3$	114.478	36.2372	98.336	0.36	3.159
Ag	84.174	30.31102	81.1878	0.34	2.777

Table 6 – Bulk modulus B, shear modulus G, Young's modulus E (GPa); K and ν are dimensionless quantities. Disordered Au-Ag alloys

Phase	B	G	E	ν	K
$AgAu_3$	141.831	29.183	81.929	0.40	4.860
$AuAg_3$	45.265	18.558	48.978	0.32	2.439

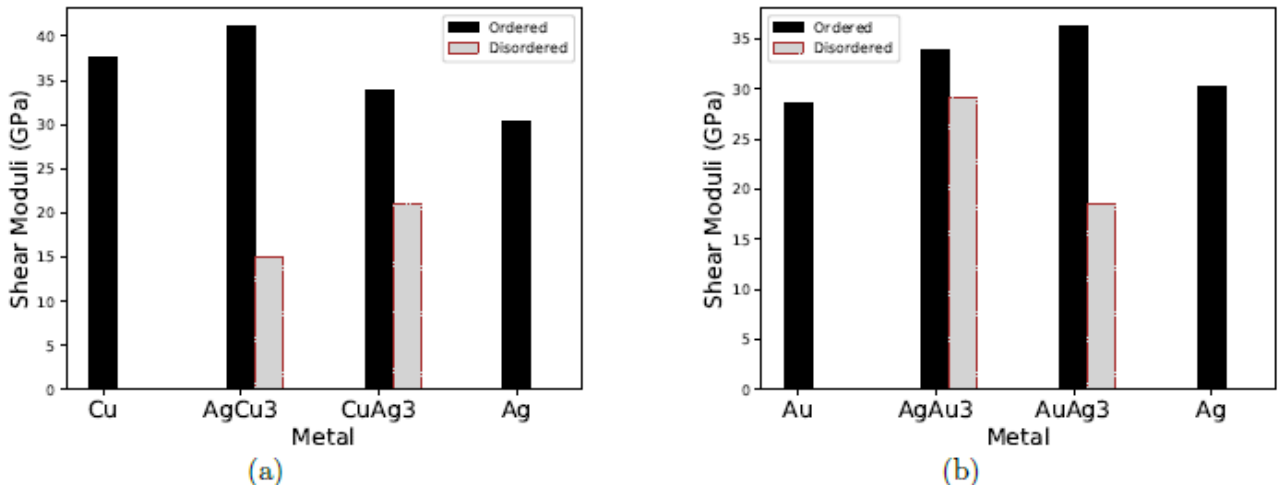

Figure 2 – Comparison of shear modulus of ordered and disordered alloys: a) Cu-Ag; b) Au-Ag

From the simulations, we were able to get the value of bulk modulus, shear modulus, elastic constants and lattice parameter of the metals and their alloys. The Young's modulus, *E*, is calculated using Eq. (10) while Poisson's ratio is obtained using Eq. (11). The Pugh's ratio is obtained by dividing bulk modulus to shear modulus. The results of our computations are displayed in tables 2 , 3, 4, 5 and 6.

Table 7 – The percentage of decrease of elastic properties of disordered alloys when compared with ordered counterparts

Alloy	Bulk Modulus	Shear Modulus	Young's Modulus
$AgCu_3$	6.501	63.419	61.121
$CuAg_3$	5.053	38.131	36.115
$AgAu_3$	7.723	13.851	13.459
$AuAg_3$	60.459	48.790	50.193

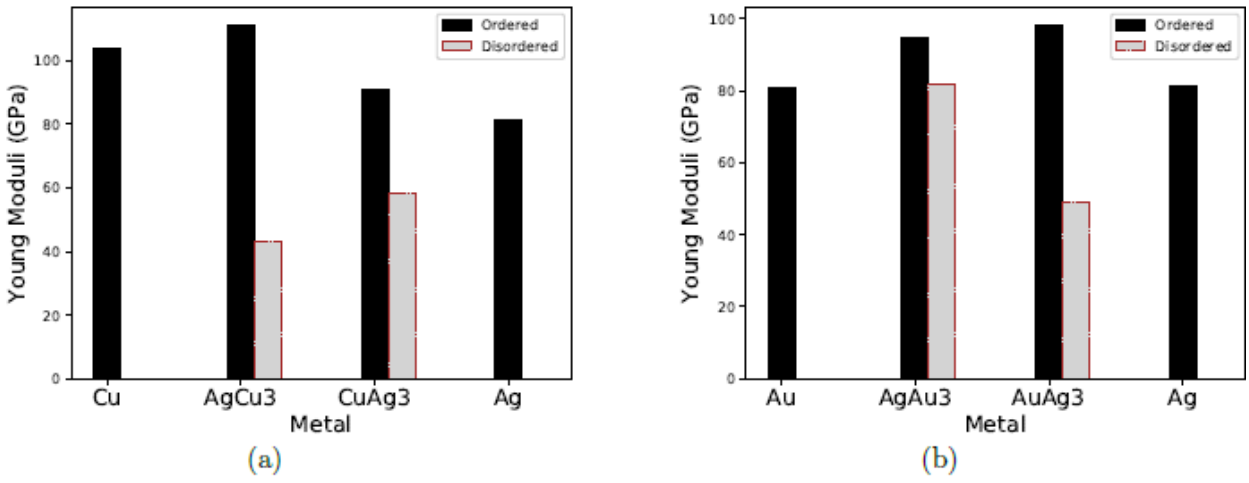

Figure 3 – Comparison of Young's modulus of ordered and disordered alloys:
a) Cu-Ag; b) Au-Ag

Fig. 1 shows bulk moduli of ordered metals and it's disordered counterpart. Fig. 2 presents shear moduli while Fig. 3 shows Young's moduli of ordered and disordered alloys. The bulk, shear and Young's moduli of the disordered alloys showed a decreasing trend when compared to ordered counterparts (See table 7). When we see the percentage of decrease in bulk moduli all the values are less than 8% except the value for $AuAg_3$ which is 60.459%. The very high percentage of decrease could be attributed to the fact that optimization was not achieved in the structure of disordered $AuAg_3$.

The values of C_{11}, C_{12} and C_{44} for ordered alloys is higher than the disordered ones. The influence of chemical disorder on elastic constants is higher on C_{11} and C_{44} while it is minimal on C_{12}. Poisson's ratio and the lattice parameter (a) of disordered alloys are greater than ordered counterparts. The bulk, shear and Young's moduli of the ordered alloys are higher than their disordered counterparts. Generally speaking, ductility of the ordered alloys is less than disordered counterparts. It can also be seen that the Poisson's ratio for the disordered alloys is slightly higher in comparison to the ordered metals.

4 Conclusions

We present computer simulation results of the mechanical properties of Cu-Ag and Au-Ag alloys based on Sutton-Chen semi-empirical model. The focus was to investigate the influence of chemical disorder on some mechanical properties of the alloys under study. The main observations of the study can be summarized in the following points:

1) In all the investigated alloys, the respective bulk, shear and Young's moduli of the ordered alloy is greater than the disordered alloy. In most cases, the ductility of the disordered alloys is greater than the ordered counterpart.

2) All the alloys of Cu-Ag and Au-Ag considered on this investigation have good ductility coefficient ($K > 1.75$). In general, chemically disordered alloys are more ductile than ordered counterparts.

3) Chemical disorder influences highly shear modulus followed by Young's modulus. The influence of chemical disorder on bulk modulus is insignificant in most cases.

4) The influence of chemical disorder on the elastic contents C_{11} and C_{44} is significant while on C_{12} it's influence is small.

5) All the alloys investigated here satisfy the conditions of stability given in the inequalities given by Ineq. (5).

Thus, the study confirms that chemical disorder of alloys has significant influence on shear and Young's moduli while the influence on bulk modulus is insignificant. It further confirms that it's influence on elastic constants is also significant, especially on C_{11} and C_{44}.

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