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Embedded atom method for elastic constants of iridium binary alloys (at room temperature)

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The elastic constants are paramount to determine the strength of alloys. The elastic constants of M -Ir, M_3 -Ir, and M -Ir₃ where M represents Cu, Au, Ni, Ag, Pt, Al, Pd and Rh were computed at room temperature using the embedded atom method (EAM) and the alloy mixing potentials. The potential parameters of the selected pure metals were fitted to the experimental values to compute some properties of Ni-Al, Ni₃-Al, Ni-Al₃, Cu-Au, Cu₃-Au and Cu-Au₃, and by comparing the experimental data with our predictions, the employed potential predicted some results in reasonable agreement to available experimental data with discrepancies in some cases, and these discrepancies linked to the dependence of the computed elastic constants on the fitting parameters. The potential with the metallic parameters was used as alloy parameters in computing the elastic constants, bulk modulus, and the shear modulus of the iridium binary alloy. It was generally observed that, the selected metals improve the ductility of Iridium with the highest value, recorded for Pd-Ir, and consequently the minimum value for Al-Ir, and Rh-Ir which characterized them to be ductile. The balance orders for the binary alloys were provided through the formation enthalpy.

Keywords: Ductility; alloy mixing potentials; bulk modulus; shear modulus.

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1. Introduction

Iridium (Ir) is one of the most important elements among the nine rarest elements of the platinum group metals (PGMs). It usually occurs in nature as an uncombined element or natural alloys. The PGMs are immensely important in numerous technologies, but the experimental and computational data of the properties of their binary alloy still contain many gaps. Interest in PGMs is driven by their essential role in a wide variety of industrial applications, but the high cost is a challenging issue. Iridium (Ir) is one of the most important elements among the nine rarest elements of

T. H. Akande et al.

the PGMs. It normally happens in nature as an uncombined detail or in natural alloys. The PGMs are immensely vital in several technologies, however, the experimental and computational information of their binary alloys residences nonetheless contain many gaps. Interest in PGMs is driven by way of their essential function in an extensive application, but the excessive price is a tough issue. The primary software of PGMs is in catalysis, where they are fundamental components within the chemical, petroleum, and car industries. They are also top as alloying additives in aeronautics and electronics packages. The use of platinum alloys in the earrings enterprise additionally accounts for a meaningful percentage of its worldwide consumption.¹

Advances in the first-principles methodology for the computation of materials properties open the likelihood to supplement the trial information by computational outcomes. In the literary works, numerous ongoing examinations present computation of PGM composite structures.² However, the vast majority of these investigations think about a predetermined number of structures, at only a couple of stoichiometries for the binary alloys or a few of them.³ Past examinations executed have provided useful information on the binary systems of explicit metals-hafnium, rhenium, rhodium, ruthenium and technetium.⁴ The ability to distinguish new composite stages is a key to the properties of PGM compounds and their usage in new applications, or as a diminished expense or higher-action substitutes in new applications.⁵

For instance, the platinum–iridium (Pt–Ir) combinations are generally utilized as the defensive coatings to expand the administration life of the form in glass shaping cycle and this glass shaping cycle has given an incredible potential to the creation of glass optical segments with ease and substitutes the conventional machining cycle to yield glass lenses.⁶ Several materials can be used as the protective coating on the mold surface such as diamond-like carbon (DLC), Ir–Re alloy and Ir–Pt alloy.⁷

The elastic constants as the major determinant of structural properties play an important role in determining the response of a material to applied stress. Atoms are displaced from their stable positions when twisted by interatomic powers. For any little stress, the applied forces correspond to the relocation of the atoms. In describing elastic properties, crystals are considered to be a homogeneous medium rather than just a periodic array of atoms.⁸

The embedded atom method (EAM)⁹ used for calculating the elastic constants of metals can also be used to predict the existence and properties of new materials. Through the theoretical search for new materials, an interesting and vital area of research is to examine iridium binary systems' elastic constants which correlate with the strength. These alloys are likely to be a good candidate for new structural materials and good substitutes in alloy processes if not brittle. Maintaining the high strength of metallic materials by alloying these metals can improve their ductility. It has been observed in the literature that the use of pure metals is very rare, instead, they are used in form of alloy since their properties have been altered to suit the purpose of interest. Many experimental and theoretical research works on elastic

constants have been concentrated on Au–Pd, Ag–Pt, Cu–Au and Ni–Al alloy systems and leaving others unexplored.

Material science has uncovered that the versatile constants C_{ij} contains heaps of more indispensable data that can be accomplished starting from the ground state complete energy estimations. The elastic constants decide the reaction of crystal to outer forces as described by the bulk modulus, shear modulus, Young's modulus and Poisson's proportion which assume a ceaseless part in deciding the quality of materials.¹⁰

Some EAM potential utilized the total form of the embedding function based on Mayer function and the equation of state to describe the properties of metals.¹¹ Potentials for Ni–Al alloy have been constructed and the equation of states with the phonon dispersions is calculated.¹² Iridium (Ir), Platinum (Pt), Rhodium (Rh) and Palladium (Pd) are future candidates of new superalloys and some of these metals have high melting points but the bone of contention is the use of these metals at equilibrium temperature.¹³

Foiles¹⁴ constructed an interatomic potential for Ni–Cu and Ag–Cu alloy systems using the EAM. Landa *et al.* developed the glue-potential for the Al–Pb immiscible alloy system by applying the force-matching method (FMM) and presented a hypothetical Pb_3Al intermediate alloy phase to fit the potential function for the Al–Pb alloy system to its properties.¹⁵ The bulk modulus of V, Cr, Mo and Fe and their binary alloys have been presented and the bulk to shear modulus ratio was used to characterize the toughness of the selected metals.¹⁶ The EAM removes the difficulties of calculating the ground state properties of pure metals such as vacancy forming energy, elastic constants, and describing volumes involving defect through a simple pair potential. At the moment, no known analytical theory of physics can deal with real systems such as alloys. However, computational physics (atomistic simulation) through the use of EAM has the advantage of being able to determine the alloys that are worthy of experimental attention and to identify candidates for possible substitution alloying. In this research, therefore, the calculation efforts centered on computation of elastic constants of the iridium binary alloy systems at room temperature through atomistic simulations and to determine the bulk and shear modulus ratio to investigate their strength.

2. Theory

Each atom in metal is embedded into the electron gas created by any other atoms and the total energy of the atom is written as follows:

$$E_{\text{tot}} = \sum_i F_i(\rho_i) + \frac{1}{2} \sum_{i,j} \phi_{ij}(r_{ij}), \quad (1)$$

where

$$\rho_i = \sum_{j \neq i} f_{ij}(r_{ij}). \quad (2)$$

T. H. Akande et al.

The parameter $F_i(\rho_i)$ is the energy to insert an atom into the local environment of electron provided by the remainder of the atoms, ϕ_{ij} is an electrostatic two-body interaction between atoms i and j , and $f_{ij}(r_{ij})$ is the local electron density.

The electron density employed in this work takes exponential form in the following equation:

$$f(r_o) = f_o \exp\left[-\beta\left(\frac{r}{r_o} - 1\right)\right], \quad r \leq r_c \quad (3)$$

and the potential between atoms i and j is calculated as follows:

$$\phi^{ij}(r_o) = \phi_o \exp\left[-\gamma\left(\frac{r}{r_o} - 1\right)\right], \quad r \leq r_c, \quad (4)$$

where r_o is the equilibrium distance, r is the distance and r_c represents the cut-off distance.

The equilibrium embedding function ($F(\rho_o)$) is given in the following equation:

$$F(\rho_o) = -E_c \left[1 - \frac{\alpha}{\beta} \ln\left(\frac{\rho}{\rho_o}\right)\right] \left[\frac{\rho}{\rho_o}\right]^{\frac{\alpha}{\beta}} - \Phi_o \left[\frac{\rho}{\rho_o}\right]^{\frac{\gamma}{\beta}}, \quad (5)$$

where

$$\rho_o = 12f_o \text{ and } \Phi_o = 6\phi_o. \quad (6)$$

To determine the two adjustable parameters f_o and ϕ_o for each metal, Eq. (7) was used.

$$f_o = \frac{E_c}{\Omega_o} \text{ and } \phi_o = \frac{E_c}{6}, \quad (7)$$

$$\alpha = 3 \left(\frac{\Omega_o B}{E_c}\right)^{\frac{1}{2}}, \quad (8)$$

$$\beta = \left(\frac{15E_c \Omega_o G}{E_v(E_v + E_c)}\right)^{\frac{1}{2}}, \quad (9)$$

$$\gamma = \left(\frac{15\Omega_o G(E_c + E_v)}{E_c E_v}\right)^{\frac{1}{2}}. \quad (10)$$

In Eqs. (3)–(10), E_c , is the cohesive energy; Ω_o , is the atomic volume; B is the bulk modulus; G , is the shear modulus; E_v , is the vacancy formation energy and α , β and γ represent the model parameters which can also be treated as adjustable parameters.

Therefore, the bulk modulus B and the shear modulus G are determined from Eqs. (11) and (12), respectively, where C_{11} , C_{12} and C_{44} represent the cubic elastic constants.

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

$$G = \frac{1}{5}(C_{11} - C_{12} + 3C_{44}). \quad (12)$$

Embedded atom method for elastic constants of iridium binary alloys

The atomic volume

$$\Omega_o = \frac{a_o^3}{4}. \quad (13)$$

For the elastic constants or for any defect calculation in which the relaxations are small, the exact choice of the cut-off radius r_c has no significant effect as long as the cut-off occurs within the gap between first and second neighbors.¹⁷

2.1. Alloy mixing potentials

Many processes are required in predicting properties of the alloy and several ideas have been used to predict properties such as optical, electrical, thermal, structural and elastic properties for metals and their alloys.

Here, the alloys pair potential was calculated through the mixing rule¹⁸ as follows:

$$\phi_{ab}(r_o) = \frac{1}{2} \left[\frac{f_a(r_o)}{f_b(r_o)} \phi_{aa}(r_o) + \frac{f_b(r_o)}{f_a(r_o)} \phi_{bb}(r_o) \right]. \quad (14)$$

From Eq. (3),

$$f'(r_o) = \frac{-\beta r}{r_o^2} f(r_o) \quad (15)$$

and

$$f''(r_o) = \frac{-\beta r}{r_o^2} \left[f'(r_o) - \frac{2}{r_o} f(r_o) \right]. \quad (16)$$

From Eq. (4)

$$\phi'(r_o) = \frac{-\beta r}{r_o^2} \phi(r_o), \quad (17)$$

$$\phi''(r_o) = \frac{-\beta r}{r_o^2} \left[\phi'(r_o) - \frac{2}{r_o} \phi(r_o) \right]. \quad (18)$$

From Eq. (5)

$$F'(\rho_o) = -E_c \left\{ \left(\frac{\alpha}{\beta} \right)^2 \ln \left(\frac{\rho}{\rho_o} \right) \left[\frac{\rho^{\frac{\alpha}{\beta}}}{\rho_o^{\left(\frac{\alpha}{\beta}+1\right)}} \right] \right\} + \Phi_o \frac{\gamma}{\beta} \left[\frac{\rho^{\frac{\gamma}{\beta}}}{\rho_o^{\left(\frac{\gamma}{\beta}+1\right)}} \right], \quad (19)$$

$$F''(\rho_o) = E_c \left\{ 1 + \left(\frac{\alpha}{\beta} + 1 \right) \ln \left(\frac{\rho}{\rho_o} \right) \left(\frac{\alpha}{\beta} \right)^2 \left[\frac{\rho^{\frac{\alpha}{\beta}}}{\rho_o^{\left(\frac{\alpha}{\beta}+2\right)}} \right] \right\} + \Phi_o \frac{\gamma}{\beta} \left(\frac{\gamma}{\beta} + 1 \right) \left[\frac{\rho^{\frac{\gamma}{\beta}}}{\rho_o^{\left(\frac{\gamma}{\beta}+2\right)}} \right]. \quad (20)$$

T. H. Akande et al.

Also, from Eq. (14)

$$\begin{aligned} \phi'_{ab}(r_o) &= \frac{f_a(r_o)}{f_b(r_o)} \phi'_{aa}(r_o) + \frac{[f_b(r_o)f'_a(r_o) - f_a(r_o)f'_b(r_o)]}{[f_b(r_o)]^2} \phi_{aa}(r_o) + \frac{f_b(r_o)}{f_a(r_o)} \phi'_{bb}(r_o) \\ &+ \frac{[f_b(r_o)f'_a(r_o) - f_a(r_o)f'_b(r_o)]}{[f_a(r_o)]^2} \phi_{bb}(r_o) \end{aligned} \quad (21)$$

and

$$\phi''_{ab}(r_o) = B_1 + B_2 + B_3, \quad (22)$$

where

$$\begin{aligned} B_1 &= \frac{f_a(r_o)}{f_b(r_o)} \phi''_{aa}(r_o) + \frac{2[f_b(r_o)f'_a(r_o) - f_a(r_o)f'_b(r_o)]}{[f_b(r_o)]^2} \phi'_{aa}(r_o) \\ &+ \left\{ \frac{B_{1a} - B_{1b}}{[f_b(r_o)]^4} \right\} \phi_{aa}(r_o). \end{aligned} \quad (23)$$

In Eq. (23)

$$B_{1a} = [f_b(r_o)]^2 [f_b(r_o)f''_a(r_o) - f_a(r_o)f''_b(r_o)], \quad (24)$$

$$B_{1b} = [f_b(r_o)f'_a(r_o) - f_a(r_o)f'_b(r_o)][2f_b(r_o)f'_b(r_o)], \quad (25)$$

$$B_2 = \frac{f_b(r_o)}{f_a(r_o)} \phi''_{bb}(r_o) + \frac{2[f_a(r_o)f'_b(r_o) - f_b(r_o)f'_a(r_o)]}{[f_a(r_o)]^2} \phi'_{bb}(r_o), \quad (26)$$

$$B_3 = \left\{ \frac{[f_a(r_o)]^2 [f_a(r_o)f''_b(r_o) - f_b(r_o)f''_a(r_o)] - [f_a(r_o)f'_b(r_o)] - f_b(r_o)f'_a(r_o)][2f_a(r_o)f'_a(r_o)]}{[f_a(r_o)]^4} \right\} \phi_{bb}(r_o). \quad (27)$$

Note: $B_1, B_{1a}, B_{1b}, B_2, B_3$ are ordinary constants; $\phi_{ab}(r_o)$ is the pairing between atoms a and b ; $\phi_{aa}(r_o)$ is the pairing of atoms a and a while $\phi_{bb}(r_o)$ is the pairing of atoms b and b . $f_a(r_o)$ and $f_b(r_o)$ are the electron densities of atoms a and b respectively.

By substituting the alloy potential parameters for the metallic parameters, and then set

$$\begin{aligned} Y_a &= \frac{a_{o(ab)}^2}{2\Omega_{o(ab)}} \left[\left\{ \phi''_{ab}(r_o) - \frac{1}{r_{o(ab)}} \phi'_{ab}(r_o) \right\} + 2[F'(\rho_{oa}) + F'(\rho_{ob})] \right. \\ &\times \left. \left\{ [f''_a(r_o) + f''_b(r_o)] - \frac{1}{r_{o(ab)}} [f'_a(r_o)f'_b(r_o)] \right\} \right]. \end{aligned} \quad (28)$$

Again, we set

$$Y_b = \frac{8a_{o(ab)}^2}{\Omega_{o(ab)}} [(f'_a(r_o))^2 + (f'_b(r_o))^2][F''(\rho_{oa}) + F''(\rho_{ob})], \quad (29)$$

Embedded atom method for elastic constants of iridium binary alloys

where Y_a and Y_b are constants, $F(\rho_o a)$ is the embedding energy of atom a and $F(\rho_o b)$ is the embedding energy of atom b . Hence, the alloy elastic constants is computed using

$$C_{11} = Y_a + Y_b, \quad (30)$$

$$C_{12} = 0.5 * Y_a + Y_b, \quad (31)$$

$$C_{44} = 0.5 * Y_a. \quad (32)$$

For cubic crystal, it has been observed from literatures that with symmetry, we have three independent elastic variables in C_{ij} which are C_{11} , C_{12} and C_{44} and the elastic constants for cubic crystal obey the following mechanical stability¹⁹:

$$C_{11} > 0; \quad C_{11} > |C_{12}|; \quad C_{11} + 2C_{12} > 0; \quad C_{44} > 0. \quad (33)$$

The lattice constants for the alloys were computed using the following equations:

$$a_{o(ab)} = \frac{C_1 a_1 + C_2 a_2}{C_1 + C_2}, \quad (34)$$

where C_1 , C_2 are the concentrations of the first and second atom. a_1 and a_2 represent the lattice constants of the first and the second atom, respectively.

3. Results and Discussion

The EAM with a combination of estimated and optimized parameters was used to provide a theoretical description of the iridium binary alloy systems of the selected FCC metals through atomistic simulations which offer the possibility of characterizing alloying processes. Some of the binary alloys covered are well known in the literature, while some are yet to be described. This work has undertaken a thorough examination of iridium binary alloys with selected FCC metals, using the EAM. The potential parameters of the selected pure metals were fitted to the experimental values, including their lattice parameters, cohesive energies, and vacancy formation energies. We calculate the elastic constants of the selected alloys, and by comparing experimental data with our predictions, we discovered the employed potential predicted some results in reasonable agreement with available experimental data with discrepancies in some cases, and these discrepancies linked to the dependence of the computed elastic constants on the fitting parameters.

The parameters were chosen for the calculation of the three versatile elastic constants C_{11} , C_{12} and C_{44} of the binary systems are equivalent to that of its unadulterated metals. To decide these boundaries, the experimental values of the lattice constants, cohesive energy and vacancy formation energy, are fitted for the bulk alloys of M -Ir, M_3 -Ir and M -Ir₃, where M represents Cu, Au, Ni, Ag, Pt, Al, Pd and Rh. The fitting strategy was performed at the differed cut-off separation of $r_c \leq 1.6r_o$ for the metals. To compute the alloys parameters, the derivatives of the embedding energy, electron density, two body cooperation potential, and the alloy mixing potential were filled in for the metallic parameters, and the elastic constants C_{11} , C_{12} and C_{44} were figured.

T. H. Akande et al.

Table 1. Input parameters a_o , E_c , E_v and calculated model parameters f_o , ϕ_o , α , β and γ .

Metals	a_o (Å)	E_c (eV)	E_v (eV)	f_o (eV)	ϕ_o (eV)	α	β	γ
Cu	3.615 ^a	3.54 ^a	1.30 ^b	0.30	0.59	5.09	5.81	7.94
Ag	4.090 ^a	2.85 ^a	1.10 ^b	0.17	0.47	5.91	5.96	8.26
Ni	3.520 ^a	4.45 ^a	1.70 ^d	0.41	0.74	4.98	6.41	8.86
Pt	3.920 ^a	5.77 ^a	1.60 ^d	0.38	0.96	6.44	6.70	8.56
Au	4.080 ^a	3.93 ^a	0.90 ^b	0.23	0.66	6.36	6.67	8.20
Pd	3.890 ^a	3.91 ^a	1.54 ^d	0.27	0.65	6.43	5.90	8.23
Al	4.050 ^a	3.39 ^a	0.67 ^c	0.20	0.56	4.67	7.55	9.04
Ir	3.840 ^a	6.94 ^a	1.97 ^b	0.14	0.34	12.04	8.86	17.46
Rh	3.800 ^a	5.75 ^a	1.71 ^d	0.42	0.96	6.00	12.05	14.54

Notes: ^aRef. 20. ^bRef. 21. ^cRef. 22. ^dRef. 23.

Table 1 presents the inputs and calculated model parameters used in fittings.

The attributes of the embedding energy of the nine metals are presented in Fig. 1 and it is evident from the curves that the embedding energies have a positive repeating pattern shown by least characteristics which increase on the entire region by the solvent electron density particularly for Iridium metal with evenness of $\frac{\rho}{\rho_o} = 1$.

Figure 2 shows the total energy curves versus distance for a portion of the chosen binary systems. The figure depicts how the constancy energy of the alloy is being overpowered by both the pair potential and the embedding energy.

Table 2. Cubic elastic constants C_{11} , C_{12} and C_{44} , bulk modulus B , and shear modulus G of the binary alloys from experiments (at 0 K). Elastic constants were obtained from an approximation of the derivative of the embedding energy, electron density and the potential. All results are given in GPa except the lattice constants a_o .

System	a_o (Å)	C_{11}	C_{12}	C_{44}	B	G	B/G
Ni–Al	3.79	258.96	131.60	63.68	174.00	63.68	2.73
	3.785 ^e	199 ^f	137 ^f	116 ^f	158 ^g		
Ni ₃ –Al	3.65	267.16	135.78	65.69	179.57	65.90	
	3.573 ^e	230 ^h	150 ^h	131 ^h	177 ^g		
Ni–Al ₃	3.92	251.23	127.66	61.79	168.85	61.29	
	3.918 ^e						
Cu–Au	3.85	241.54	121.01	60.27	161.19	60.27	2.67
	3.84 ⁱ						
Cu–Au ₃	3.96	235.60	118.03	58.78	157.22	58.79	
	3.98 ^a	189 ^j	155 ^j	47 ^j	166 ^j		
Cu ₃ –Au	3.73	247.78	124.14	61.82	165.34	61.82	
	3.74 ^a	189 ^j	132 ^j	74 ^j	150 ^j		

Notes: ^aRef. 20. ^eRef. 24. ^fRef. 25. ^gRef. 26. ^hRef. 27. ⁱRef. 28. ^jRef. 29.

Table 2 consists the information on the cubic elastic constants C_{11} , C_{12} and C_{44} , bulk modulus B and shear modulus G of the binary alloys from experiments (at 0 K). The available experimental values are indicated in the indicated references.

Embedded atom method for elastic constants of iridium binary alloys

Table 3. Cubic elastic constants C_{11} , C_{12} and C_{44} , bulk modulus B and shear modulus G of the Iridium binary alloys from EAM potential (at 0 K). Elastic constants were obtained from an approximation of the derivative of the embedding energy, electron density and the potential. All results are given in GPa except the lattice constants a_o .

System	$a_o(\text{\AA})$	C_{11}	C_{12}	C_{44}	B	G	B/G
Cu-Ir	3.73	152.20	80.86	35.67	104.64	35.67	2.93
Cu ₃ -Ir	3.62	153.46	81.56	35.95	105.53	35.95	
Cu-Ir ₃	3.78	150.94	80.16	35.39	103.76	35.39	
Ag-Ir	3.97	214.48	118.48	48.00	150.48	48.00	3.13
Ag ₃ -Ir	4.03	211.92	117.02	47.45	148.66	47.45	
Ag-Ir ₃	3.90	217.09	119.97	48.56	152.34	48.56	
Pt-Ir	3.88	432.25	235.99	98.13	301.41	98.13	3.13
Pt ₃ -Ir	3.90	430.87	235.19	97.83	300.41	97.83	
Pt-Ir ₃	3.86	433.64	236.79	98.43	302.41	98.43	
Au-Ir	3.96	113.66	69.00	22.33	83.89	22.33	3.76
Au ₃ -Ir	4.02	112.77	68.38	22.20	83.77	22.20	
Au-Ir ₃	3.90	114.54	69.63	22.46	84.60	22.46	
Al-Ir	3.95	202.97	103.09	49.94	136.39	49.94	2.73
Al ₃ -Ir	4.00	201.16	102.17	49.50	135.17	49.50	
Al-Ir ₃	3.89	204.81	104.03	50.39	137.63	50.39	
Rh-Ir	3.82	409.77	207.58	101.10	274.98	101.10	2.72
Rh ₃ -Ir	3.81	410.79	208.10	101.35	275.66	101.35	
Rh-Ir ₃	3.83	408.76	207.07	100.85	274.30	100.85	
Pd-Ir	3.87	126.77	82.55	22.11	97.29	22.11	4.40
Pd ₃ -Ir	3.88	126.62	82.42	22.10	97.15	22.10	
Pd-Ir ₃	3.85	126.92	82.69	22.12	97.43	22.12	
Ni-Ir	3.68	203.78	106.99	48.39	139.25	48.39	2.28
Ni ₃ -Ir	3.60	207.58	109.01	49.29	141.86	49.29	
Ni-Ir ₃	3.76	200.11	105.05	47.53	136.74	47.53	

Notes: In Table 3, the predicted B/G ratios revealed that all the Iridium binary alloys are ductile with a high value of ductility limit.

Table 4. Equilibrium enthalpy of formation and mixing.

Alloy	ΔH^f kJ/mol at.	ΔH kJ/mol
Al _{0.49} Ir _{0.51}	-60.9740	-174.240
Ni _{0.52} Ir _{0.48}	-2.2440	-5.523
Cu _{0.01} Ir _{0.99}	0.0040	0.479
Rh _{0.01} Ir _{0.99}	0.0245	2.490
Pd _{0.99} Ir _{0.01}	0.2350	24.345
Ag _{0.99} Ir _{0.01}	0.6010	65.487
Pt _{0.99} Ir _{0.01}	0.0140	1.510
Au _{0.99} Ir _{0.01}	0.4770	53.363

Notes: Table 4 predicted the equilibrium enthalpy of formation ΔH^f and mixing ΔH . The order of stability as predicted is Al_{0.49}Ir_{0.51} > Ni_{0.52}Ir_{0.48} > Cu_{0.01}Ir_{0.99} > Pt_{0.99}Ir_{0.01} > Rh_{0.01}Ir_{0.99} > Pd_{0.99}Ir_{0.01} > Au_{0.99}Ir_{0.01} > Ag_{0.99}Ir_{0.01}.

T. H. Akande et al.

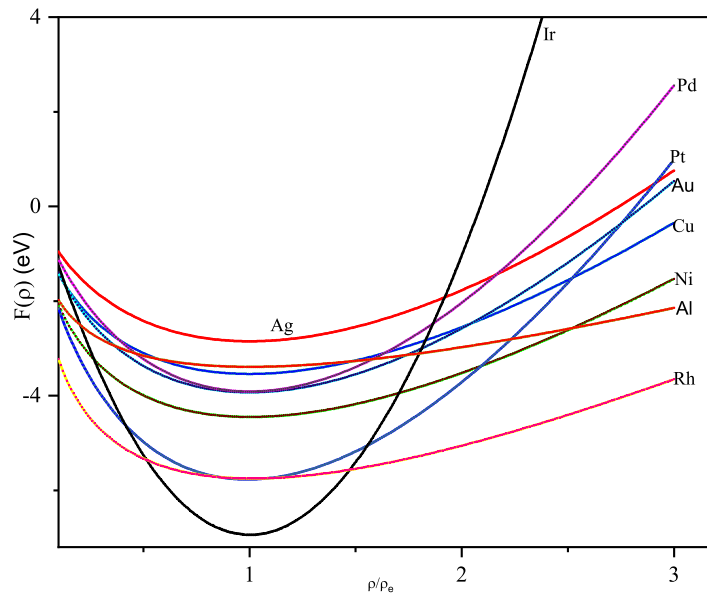


Fig. 1. (Color online) Characteristics embedding energy curves of the selected metals.

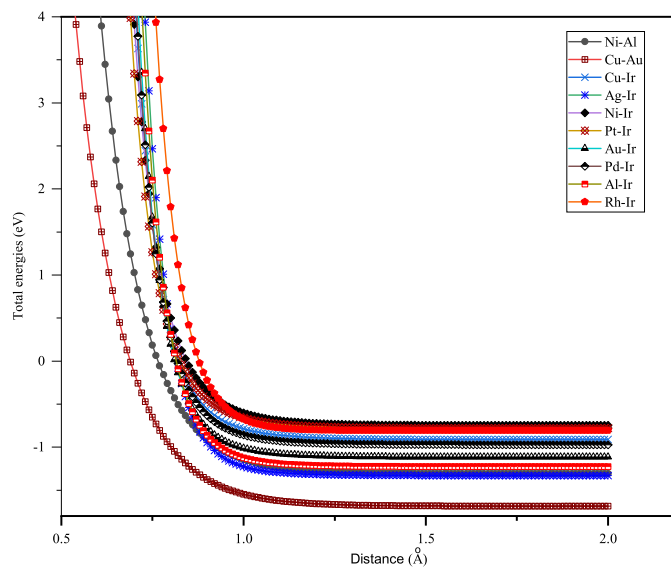


Fig. 2. (Color online) Characteristics of the total energy curves for some selected alloys.

In Fig. 3, we have the comparison of the B/G and Poisson's ratios of iridium with some selected iridium alloys. Generally, Fig. 3 shows that the addition of the selected FCC metals improves the ductility of Iridium with the highest value recorded for Pd-Ir and the minimum value for Al-Ir and Rh-Ir.

Embedded atom method for elastic constants of iridium binary alloys

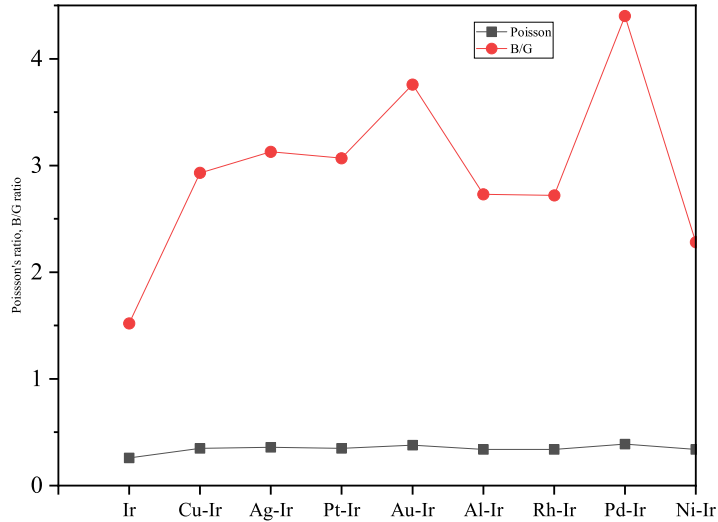


Fig. 3. (Color online) Iridium addition to other metals.

The alloy mixing rule in the model (Eq. (15)) was applied to compute the elastic constants of the binary alloy systems. The lattice constant of the binary alloy systems was also predicted. These properties are very essential in material selection and provide insight into how manufacturers can achieve standard materials.

To obtain the properties of the selected FCC metals, Eqs. (1)–(6) that contain accurate interatomic potentials were used. The parameters in the EAM model were computed using Eqs. (9)–(11).

Cut-off radius r_c was chosen for the two atoms and the position of the two atoms was adjusted to have the first atom on the face and the second atom at the corner and vice-versa as FCC crystal. We then compute the elastic constants C_{ij} of the binary alloys by fitting the embedding function (ρ_o), electron density $f(r_o)$ and the pair-potential $\phi(r_o)$ of the EAM.

4. Conclusion

The elastic property of material plays an important role as parameters that matched the microscopic behaviors of materials with macroscopic mechanical behaviors using information about the crystal stability and stiffness. This work on Iridium binary alloy systems helps us to understand the role of alloying elements in providing unique materials for various applications in the industries. It is interesting to know that alloying and process modifications can change the properties of metal from low to high strength materials for higher temperature applications. The computed elastic properties using the EAM and the alloy mixing potentials give results that reasonably agree with experimental values in some cases. It was observed that majority of the selected metals increase the strength of Ir metal when alloyed.

T. H. Akande et al.

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