First-principles investigation of phase stability, elastic and thermodynamic properties in $L1_2$ $Co_3(Al,Mo,Nb)$ phase

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Abstract: First-principles calculations have been performed to investigate the phase stability, elastic, and thermodynamic properties of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ with the L1_2 structure. Calculated elastic constants show that $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ is mechanically stable and possesses intrinsic ductility. It is found that the shear and Young's moduli of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ are smaller than those of $\text{Co}_3(\text{Al},\text{W})$. Calculated density of states indicate the existence of covalent-like bonding in $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$. Temperature-dependent thermodynamic properties of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ can be described satisfactorily using the Debye-Grüneisen approach, including entropy, enthalpy, heat capacity and linear thermal expansion coefficient, showing their significant temperature dependences. Furthermore the obtained data can be employed in the modeling of thermodynamic and mechanical properties of Co-based alloys to enable the design of high temperature alloys.

Keywords: A. Intermetallics; B. Phase stability; B. Elastic properties; B. Electronic structure; B. Thermodynamic properties; E. ab-initio calculations

1. Introduction

Ni-based superalloys strengthened by γ' precipitates in $L1_2$ structure have been widely used as the high-temperature materials for industrial gas turbines, aircraft engines, and reactors [1, 2]. However, these superalloys cannot satisfy the increasing demand for materials with higher-temperature capabilities. It is found that Co-based alloys display superior hot corrosion resistance at high temperatures compared to Ni-based alloys [2]. Nevertheless, the traditional Co-based alloys exhibit a lower strength at high temperatures with respect to Ni-based alloys, where Ni-based alloys are strengthened by the precipitation hardening effect caused by the formation of γ' $\text{Ni}_3(\text{Al,Ta})$ phase [3]. However, the γ' phase has not been applied in Co-based commercial alloys. Interest in Co-based alloys has been fueled because of the discovery of the $L1_2$ ordered $\text{Co}_3(\text{Al,W})$ precipitate [4]. The Co-Al-W-base alloys with $\gamma+\gamma'$ structures exhibit higher strength at elevated temperatures compared to Ni-based superalloys [4, 5]. In addition, $\text{Co}_3(\text{Ge,W})$ and $\text{Co}_3(\text{Ga,W})$ precipitates in the $L1_2$ structure have also been found in Co-Ge-W and Co-Ga-W ternary systems [6, 7]. These alloys show higher density compared with the Ni-based superalloys. Very recently, Makineni et al. [8, 9] found a new $L1_2$ ordered γ' precipitate of $\text{Co}_3(\text{Al,Mo,Nb})$ with a composition of Co-10.6 at.% Al-8.7 at.% Mo-4.8 at.% Nb in the Co-Al-Mo-Nb tungsten-free quaternary alloys. The density of this alloy is comparable to those of Ni-based superalloys. In addition, the tungsten-free alloy has higher specific proof stress compared to the Co-9 at.% Al-9.8 at.% W alloy.

In the past decade, first-principles approach has become an efficient tool for studying phase stability, mechanical, and thermodynamic properties of crystalline materials [10-12]. For example, these properties in $L1_2$ γ' - $\text{Co}_3(\text{M,W})$ ($\text{M}=\text{Al, Ge, Ga}$) have been investigated using both first-principles calculations and experiments [13-20], indicating that these γ' precipitates are

ductile and have a strengthening effect on the Co matrix. First-principles calculations also show that Ta plays a crucial role in stabilizing γ' phase for Co-Al-Mo alloys [21]. Although the γ' precipitates play an important role in the mechanical properties of the γ/γ' two-phase alloys [22], few studies have been reported for the γ' -Co₃(Al,Mo,Nb) precipitate. In the present work, we perform a first-principles study on the phase stability, elastic and thermodynamic properties of the L1₂ Co₃(Al,Mo,Nb) precipitate.

2. Theoretical methods

2.1 Crystal structure

In the unit cell of A₃B compound with the cubic L1₂ structure, A atoms located at face centers and B atoms at cube corners. In our calculations, the chemical formula is assumed as Co₂₄Al₃Mo₃Nb₂ and the nominal composition for the Co₃(Al,Mo,Nb) supercell is Co-9.375 at.% Al- 9.375 at.% Mo-6.25 at.% Nb. All the seventeen possible 2×2×2 supercell structures are generated for Co₂₄Al₃Mo₃Nb₂ using the Alloy Theoretic Automated Toolkit (ATAT) software [23]. Fig. 1 illustrates the total energies for all the seventeen supercell structures of L1₂ Co₃(Al,Mo,Nb). The structures with the lowest energy (str_1) and the intermediate energy (str_2) are chosen for further investigations of Co₃(Al,Mo,Nb), see Fig .1. Note that the str_2 with the intermediate energy can represent a special quasi-random structure (SQS) of Co₃(Al,Mo,Nb) to some extent [24, 25] (More details are provided in supplementary data). In addition, a L1₂ SQS structure constructed by Jiang [18] is also adopted for the Co₃(Al,W) compound.

2.2 Computational details

First-principles calculations on total energies, elastic constants and electronic structures of the L1₂ Co₃(Al,Mo,Nb) precipitate are performed using the projector augmented wave (PAW)

method as implemented in the Vienna *ab initio* simulation package (VASP) [26, 27]. Exchange and correlation effects are treated within the density functional theory, using the generalized gradient approximation proposed by Perdew, Burke and Enzerhof (GGA-PBE) [28]. A $8 \times 8 \times 8$ k -point mesh are used. The cutoff energy of plane wave is set as 500 eV. Convergence is judged when the energy difference between each step of the electronic iterations is less than 4×10^{-6} eV/atom. The electronic density of states (DOS) is obtained using a modified tetrahedron method [29]. The effect of spin polarization has been considered in the present work.

2.3 Elastic properties

Elastic constants are calculated using an efficient stress-strain method. The methodology involves applying a set of strains ($e = e_1, e_2, e_3, e_4, e_5$ and e_6) on a crystal. Here, e_1, e_2 , and e_3 refer to normal strains, and e_4, e_5 , and e_6 to shear strains. The corresponding stresses ($\sigma = \sigma_1, \sigma_2, \sigma_3, \sigma_4, \sigma_5$ and σ_6) for the deformed crystal are obtained from first-principles calculations. According to the Hooke's law, elastic stiffness constants are then calculated from the n set of strains and the corresponding stresses. More details are described in [30].

The quasistatic approach is used to compute the isothermal elastic constants as a function of temperature. This approach is based on the fact that the temperature dependence of elastic constants is caused mainly by the volume change of crystal at finite temperatures. The methodology can be summarized in three steps as follow: (a) calculating the elastic constants at 0 K as a function of volume; (b) predicting the volume change as a function of temperature; (c) then computing the temperature dependence of isothermal elastic constants. More details are described in [31]. Generally, the measured elastic constants at high temperatures using the resonance method are isentropic, because the system is adiabatic due to the elastic waves

traveling faster than the rate of heat conduction. For cubic crystals, the thermodynamic relations can be simplified as [10]

$$\frac{C_{11}^S}{C_{11}^T} = \frac{C_{12}^S}{C_{12}^T} = \frac{C_P}{C_V} \quad \text{and} \quad C_{44}^S = C_{44}^T, \quad (1)$$

where C_V and C_P are heat capacities at constant volume and pressure, respectively. C_{ij}^S and C_{ij}^T represent the isentropic and the isothermal elastic constants, respectively. The Voigt–Reuss–Hill approach is used to calculate the bulk (B), shear (G) and Young's (E) moduli for polycrystalline crystals [32]. Elastic anisotropy parameter is given by

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \quad (2)$$

Young's moduli along some orientations in single crystals are given by [33]

$$E_{100} = \frac{(C_{11} - C_{12})(C_{11} + 2C_{12})}{C_{11} + C_{12}} \quad (3)$$

$$E_{110} = \left\{ \frac{C_{11} + C_{12}}{(C_{11} + 2C_{12})(C_{11} - C_{12})} + \frac{1}{4} \left(\frac{1}{C_{44}} - \frac{2}{C_{11} - C_{12}} \right) \right\}^{-1} \quad (4)$$

$$E_{111} = \left\{ \frac{C_{11} + C_{12}}{(C_{11} + 2C_{12})(C_{11} - C_{12})} + \frac{1}{3} \left(\frac{1}{C_{44}} - \frac{2}{C_{11} - C_{12}} \right) \right\}^{-1} \quad (5)$$

2.4. Thermodynamic properties

Helmholtz free energy $F(V, T)$ in a solid at volume V and temperature T can be approximated by [10],

$$F(V, T) = E_0(V) + F_{vib}(V, T) + F_{el}(V, T) \quad (6)$$

where $E_0(V)$ is the static energy at 0 K without the zero point vibrational energy, $F_{\text{vib}}(V, T)$ the vibrational free energy, and $F_{\text{el}}(V, T)$ the thermal electronic free energy. $F_{\text{vib}}(V, T)$ can be estimated by the empirical Debye-Grüneisen model [34],

$$F_{\text{vib}}(V, T) = \frac{9}{8} k_B \Theta_D + k_B T \left\{ 3 \ln \left[1 - \exp \left(-\frac{\Theta_D}{T} \right) \right] - D \left(\frac{\Theta_D}{T} \right) \right\} \quad (7)$$

where k_B is Boltzmann's constant, Θ_D the volume-dependent Debye temperature, and $D(x)$ is the Debye function given by

$$D(x) = \frac{3}{x^3} \int_0^x \frac{z^3 dz}{e^z - 1} \quad (8)$$

The volume-dependent Debye temperature Θ_D is written as

$$\Theta_D = s A V_0^{1/6} \left(\frac{B_0}{M} \right)^{1/2} \left(\frac{V_0}{V} \right)^\gamma \quad (9)$$

where s is a scaling factor, A a constant $(6\pi^2)^{1/3} \hbar / k_B$, V_0 the ground state volume, M the atomic mass, and B_0 the bulk modulus. The Grüneisen constant γ is defined by

$$\gamma = \frac{1}{2} (1 + B'_0) - x \quad (10)$$

with $x=2/3$ for high temperature case and $x=1$ for low temperature case. In the present work, the high temperature value is used.

Thermal electronic contribution to Helmholtz free energy is determined by Mermin statistics $F_{\text{el}}(V, T) = E_{\text{el}}(V, T) - T S_{\text{el}}(V, T)$, where E_{el} is the internal energy and S_{el} the bare electronic entropy [35].

3. Results and discussion

3.1 Structural properties

Calculations of total energies as a function of cell volume are carried out to estimate the lattice constants of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ and $\text{Co}_3(\text{Al},\text{W})$ in the L1_2 structure. The equilibrium lattice constant is deduced from a 4-parameter Birch-Murnaghan equation of state fitting [35]. The enthalpy of formation (ΔH) is defined as the enthalpy change of the compound with respect to its constituents in their standard element reference states (SER). Calculated equilibrium lattice constants and values of ΔH at 0 K are summarized in Table 1, together with other predictions for the $\text{Co}_3(\text{Al},\text{W})$ phase [36]. It can be seen from Table 1 that the calculated lattice constant of $\text{Co}_3(\text{Al},\text{W})$ is 0.3567 nm, which agrees well with the experimental value of 0.3599 nm [4]. The ΔH value is calculated to be -12.16 kJ/mol-atom for $\text{Co}_3(\text{Al},\text{W})$, agreeing reasonably well with other theoretical result (-14.96 kJ/mol-atom) [36]. Calculated equilibrium lattice constant of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ is 0.3599 nm, which is slightly larger than that of $\text{Co}_3(\text{Al},\text{W})$.

3.2 Electronic structures

The electronic density of states (DOS) for L1_2 $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ is further calculated, which provides information on the physical basis for the phase stability of the L1_2 $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ compound. Fig. 2 shows the total and partial electronic density of states of the L1_2 $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ with the str_1 structure. It is seen that the calculated DOS of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ presents a well-defined low-energy bonding and high-energy antibonding region. A deep valley near the Fermi level called a pseudo-gap, which separates the bonding states from the antibonding states. This pseudo-gap is mainly due to the d-d hybridization among the transition metal atoms and indicates the existence of covalent-like bonding in $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$. Obviously, the phase stability of intermetallic compounds depends on the location of Fermi level [37]. The

system will be stable if the Fermi level falls in the bonding states. From Fig. 2, we see that the Fermi level is located in the bonding region of the electronic DOS, which makes the $L1_2$ $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ phase stable. The total spin up and spin down electronic DOS of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ are asymmetric, indicating that they are in ferromagnetic state. In addition, the non-zero densities around the Fermi levels occur for $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$, implying the thermal electronic contribution to free energy should be considered, especially at high temperatures.

3.3 Elastic properties

Calculated elastic properties of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$, Ni_3Al , and $\text{Co}_3(\text{Al},\text{W})$ at 0 K are presented in Table 2, together with other predictions for $\text{Co}_3(\text{Al},\text{W})$ [38]. Experimental elastic properties of Ni_3Al [39], $\text{Co}_3(\text{Al},\text{W})$ [19] and $\text{Ni}_3(\text{Al},\text{Ta})$ [19] are also listed for comparison. For cubic crystals, lattice stability requires the elastic stiffness constants that satisfy the following conditions [40]:

$$C_{44} > 0, C_{11} + 2C_{12} > 0, C_{11} - |C_{12}| > 0 \quad (11)$$

It can be seen from Table 2 that the $L1_2$ $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ is elastically stable based on Eq. (11). A good agreement is observed between calculations and measurements, in particular for Ni_3Al [39]. The elastic constants of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ with different structures are almost identical, see results for str_1 and str_2. All the shear and Young's moduli of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ are larger than those of Ni_3Al and $\text{Ni}_3(\text{Al},\text{Ta})$, but smaller than those of $\text{Co}_3(\text{Al},\text{W})$. Calculated elastic anisotropy parameter A of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ is smaller than those of Ni_3Al and $\text{Co}_3(\text{Al},\text{W})$. It was reported that the ductile/brittle behaviors of materials are related to the B/G ratio [41]. If $B/G < 1.75$, the material behaves in a brittle manner, otherwise the material in a ductile manner. On the other hand, Pettifor [42] proposed that the bonding character, which reflecting the ductile/brittle behaviors of materials, could be described by the Cauchy pressure $C_{12}-C_{44}$. For metallic bonding, the Cauchy pressure is positive. However, the Cauchy pressure is negative for

the directional bonding. It can be seen that the B/G ratio is higher than 1.75 and the Cauchy pressure is positive for $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$. Therefore, $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ is ductile in nature, and the ductility of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ is higher than that of $\text{Co}_3(\text{Al},\text{W})$.

The values of E_{110}/E_{100} and E_{111}/E_{100} are also given in Table 2. Here E_{hkl} denotes Young's modulus along the crystal direction of $[\text{hkl}]$. The values of Young's modulus are the largest in the $\langle 111 \rangle$ direction and are the smallest in the $\langle 100 \rangle$ direction for $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$, Ni_3Al , $\text{Co}_3(\text{Al},\text{W})$ and $\text{Ni}_3(\text{Al},\text{Ta})$. The E_{111} value is larger than E_{100} value by 200 GPa for $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$. This implies a strong orientation dependence for Young's modulus.

Fig. 3 shows the calculated isothermal elastic constants C_{ij}^T and isentropic elastic constants C_{ij}^S at different temperatures for the Ni_3Al phase. An agreement could be found for C_{12}^S and C_{44}^S between experiments [43] and the present calculations. For C_{11}^S , the calculated decreasing rate with increasing temperature is slightly smaller than the corresponding experimental measurements. The discrepancy found in the C_{11}^S could be attributed to the neglecting of the contributions of F_{vib} and F_{el} to these second derivatives [31]. Fig. 4 shows the calculated isentropic elastic constant C_{ij}^S , elastic properties (B , G and E), Young's modulus in the $[\text{hkl}]$ direction E_{hkl} , E_{110}/E_{100} , E_{111}/E_{100} , and elastic anisotropy parameter A for $\text{L}_{12} \text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ with the lowest energy structure (str_1) and the intermediate energy structure (str_2) at different temperatures. It can be seen that the elastic properties of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ with different structures at different temperatures are almost identical. The isentropic elastic constants of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ decrease monotonically with the increasing of temperature. The decrease in E_{111} is the fastest and the decrease of E_{100} is the slowest with increasing temperature from 300 K to 1100 K. B , G and E value of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ decrease linearly with the rising of temperature. However, the values of E_{111}/E_{100} , E_{110}/E_{100} and A of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ keep nearly constant with increasing temperature. In

$\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ phase, $[100]$ is the softest direction, which helps to explain the experimentally observed $\text{fcc}(\gamma)/\text{L1}_2(\gamma')$ two-phase microstructure with L1_2 precipitates along $\langle 100 \rangle$ directions [9, 18]. This structure is expected to lead to the excellent mechanical properties at elevated temperatures.

3.4 Thermodynamic properties

In order to verify the methodology in the present work, Fig. 5 shows the predicted thermodynamic properties at finite temperatures compared with experimental results of Al [44], Co [44], Mo [44], Nb [44] and Co_3Mo [45]. A good agreement is observed between calculations and measurements. Fig. 6 illustrates the calculated thermodynamic properties of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$. Fig.6a and Fig.6b show the temperature dependence of entropy and thermal expansion coefficient. In Fig.6c, it is shown that C_p is proportional to T^3 at temperatures near 0 K. Fig. 6d shows that the formation enthalpy of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ keeps nearly constant with respect to temperature and with the value from str_1 larger than that of str_2 by 0.4 KJ/mol-atoms. It is notable that the differences in entropy, thermal expansion coefficient and heat capacities of two structures of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ are negligible. The str_1 is the lowest energy structure, while the str_2 is the intermediate energy structure (near-SQS structure). Although str_1 and str_2 have different atomic configuration, the calculated E_0 , V_0 , B_0 , B'_0 of str_1 are very close to each other, resulting in almost identical the thermodynamic properties.

4. Conclusions

Phase stability, electronic structure, elastic, and thermodynamic properties of the L1_2 $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ phase have been obtained from first-principles calculations. A good agreement is found between the calculated results and the experimental data, which validates the present

methodologies such as the Debye model and the quasistatic approach. Calculated results indicate that $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ is mechanically stable and ductile in nature and possesses covalent-like bonding. Shear and Young's moduli of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ are larger than those of Ni_3Al and $\text{Ni}_3(\text{Al},\text{Ta})$ but smaller than those of $\text{Co}_3(\text{Al},\text{W})$. The values of E_{111}/E_{100} and A keep nearly constant with increasing temperature for $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$. The temperature has significant effects on heat capacity, entropy and linear thermal expansion coefficient of $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$. The present work provides data for the design of novel high-temperature tungsten-free Co-based alloys.

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Figures and Figure Captions:

Fig. 1. Calculated total energies for all the seventeen supercell structures of $L1_2$ $Co_3(Al,Mo,Nb)$.

The structures with the lowest energy (str_1) and the intermediate energy (str_2) are shown.

Fig. 2. Calculated total electronic density of states (TDOS) and partial electronic density of states (PDOS) for the $L1_2$ $\text{Co}_3(\text{Al}, \text{Mo}, \text{Nb})$ based on str_1. The Fermi level is shifted zero energy.

Fig. 3. Calculated isothermal elastic constants (C_{11}^T : $\square$, C_{12}^T : $\triangle$, and C_{44}^T : $\star$) and isentropic elastic constants (C_{11}^S : $\circ$, C_{12}^S : ∇ , and C_{44}^S : $\star$) for Ni_3Al at 300, 600, 900, and 1100 K in comparison with experimental data by Prihodko et al [43] (C_{11}^S : $\bullet$, C_{12}^S : $\blacktriangledown$, and C_{44}^S : $\star$).

Fig. 4. Calculated isentropic elastic constant C_{ij}^S , elastic properties (i.e., B, G and E), Young's modulus in the $[hkl]$ direction E_{hkl} , E_{110}/E_{100} , E_{111}/E_{100} , and elastic anisotropy parameter A of $L1_2$ $\text{Co}_3(\text{Al}, \text{Mo}, \text{Nb})$ with the lowest energy structure (str_1) and the intermediate energy structure (str_2) at different temperatures, respectively.

Fig. 5. Thermodynamic properties as a function of temperature for fcc Al, hcp Co, bcc Mo, bcc Nb and Co_3Mo : (a) entropy (S); (b) isobaric heat capacity (C_p); (c) enthalpy of formation (ΔH); (d) entropy of formation (ΔS). The recommended values (open symbols) are shown for Al [44], Co [44], Mo [44], Nb [44] and Co_3Mo [45].

Fig. 6. Temperature-dependent thermodynamic function of $L1_2 \text{Co}_3(\text{Al}, \text{Mo}, \text{Nb})$ with the lowest energy structure (str_1: red dashed line) and the intermediate energy structure (str_2: black solid line): (a) entropy (S); (b) linear thermal expansion coefficient; (c) isobaric heat capacity (C_p); (d) enthalpy of formation (ΔH).

Table 1

Calculated equilibrium lattice constant a (nm) and enthalpy of formation ΔH (kJ/mol-atoms) for $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$ and $\text{Co}_3(\text{Al},\text{W})$.

	Method	a	ΔH
$\text{Co}_3(\text{Al},\text{Mo},\text{Nb})\text{-str}_1$	Calc. ^a	0.3599	-11.63
$\text{Co}_3(\text{Al},\text{Mo},\text{Nb})\text{-str}_2$	Calc. ^a	0.3599	-11.25
$\text{Co}_3(\text{Al},\text{W})$	Calc. ^a	0.3567	-12.16
	Calc. ^b	0.3566	-14.96
	Expt. ^c	0.3599	-

^a This work.

^b Ref [36].

^c Ref [4].

Table 2

Calculated and experimental elastic properties, including C_{ij} , B , G and E , B/G , Cauchy pressure $C_{12}-C_{44}$, Young's modulus along the $[hkl]$ direction E_{hkl} , E_{110}/E_{100} , E_{111}/E_{100} and elastic anisotropy parameter A for $\text{Co}_3(\text{Al},\text{Mo},\text{Nb})$, Ni_3Al , and $\text{Co}_3(\text{Al},\text{W})$ at 0 K. The unit of elastic properties is GPa, and the properties of $\text{Ni}_3(\text{Al},\text{Ta})$ are listed for comparison.

	Method	C_{11}	C_{12}	C_{44}	B	G	E	B/G	$C_{12}-C_{44}$	E_{100}	E_{110}	E_{111}	E_{110}/E_{100}	E_{111}/E_{100}	A
$\text{Co}_3(\text{Al},\text{Mo},\text{Nb})\text{-str}_1$	Calc. ^a	290.7	176.6	149.6	214.6	101.7	263.4	2.11	27.0	157.2	274.0	364.2	1.74	2.32	2.62
$\text{Co}_3(\text{Al},\text{Mo},\text{Nb})\text{-str}_2$	Calc. ^a	286.7	177.1	150.7	213.6	100.5	260.6	2.13	26.4	151.4	270.3	366.1	1.78	2.42	2.75
Ni_3Al	Calc. ^a	226.9	143.5	123.1	171.3	79.8	207.3	2.15	20.4	115.7	213.8	297.9	1.85	2.57	2.95
	Expt. ^b	223	148	125	173	77	201	2.25	23	104.9	205.6	302.2	1.96	2.88	3.33
$\text{Co}_3(\text{Al},\text{W})$	Calc. ^a	304.1	184.6	175.9	224.4	114.2	292.9	1.96	8.7	164.7	302.1	418.4	1.83	2.54	2.94
	Calc. ^c	301	169	172	213	117	297	1.82	-3	179.5	308.9	406.6	1.72	2.27	2.61
	Expt. ^d	271	172	162	205	101	260	2.03	10	137.4	265.3	384.7	1.93	2.80	3.27
$\text{Ni}_3(\text{Al},\text{Ta})$	Expt. ^d	238	154	130	182	82.8	216	2.20	24	117.0	221.4	315.0	1.89	2.69	3.09

^a This work.

^b Ref [39].

^c Ref [38].

^d Ref [19].