Accurate prediction of high-temperature elastic constants of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ random alloy

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ABSTRACT

Using highly accurate ab initio molecular dynamic simulations we calculate elastic constants of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ as a function of temperature up to 1500 K and compare the results with those obtained for TiN. We analyze the variation of the material's elastic anisotropy with temperature by calculating directional Young's moduli and Poisson ratios on the (100), (110) and (111) crystallographic planes. We show that though the elastic moduli of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ strongly decrease upon heating, the elastic anisotropy increases with temperature unlike in TiN. Since several approximate approaches have recently been utilized to predict elastic constants of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ at elevated temperature we compare our results with published data and benchmark the different approximate schemes. Giving the fact that $\text{Ti}_{(1-x)}\text{Al}_x\text{N}$ is a prototypical system for hard coating applications, we conclude that the recently developed symmetry imposed force constants approach combined with the temperature dependent effective potential method is accurate and computationally cost-effective for this material class.

1. Introduction

Ab-initio calculations are useful tools in searching for functional materials. They can be utilized for data generation in materials informatics [1], or used to gain fundamental knowledge on the materials behavior [2]. Elastic constants, in general, are used to get insight into the elasto-mechanical behavior of materials [3,4]. However, predicting the elastic constants of materials at elevated temperature corresponding to the operational conditions of the cutting tools, is a challenging computational task, as it requires 1 meV/atom accuracy in energy differences to achieve 1 GPa accuracy for the constants [5]. Therefore, first-principles calculations of the materials elastic constants have recently become a competitive research field.

Ab-initio molecular dynamics (AIMD) simulations have been used to predict materials behavior at extreme conditions, like elevated temperature and high pressure [6]. Depending on the material and the property of interest, AIMD simulations can become computational expensive. Compounds, ordered structures, as well as alloys should be modelled by supercells of sufficient size to prevent spurious interactions, caused by the applied periodic boundary conditions, that alter the results of the simulations. To reduce the high computational costs, different schemes have been developed. From technical point of view, methods have been suggested to run AIMD in parallel, such that the seed

of each parallel simulation is initialised by an intelligent sampling of the phase space [7,8]. An approach to avoid the direct AIMD simulations is to perform self-consistent phonon calculations. This is done by carrying out phonon calculations within the harmonic approximation using density functional theory (DFT) followed by a sampling of the phase space based on the derived phonon dispersions. The procedure is then iterated until convergence is reached for phonon frequencies [9–11]. Another way of using the interatomic forces in reducing the computational costs, for example, in the calculations of elasto-mechanical properties of materials is to rescale the elastic constants obtained at $T = 0$ K, with the ratio of the interatomic force constants derived at $T = 0$ K and at elevated temperature. This technique has recently been utilized for $\text{Ti}_{(1-x)}\text{Al}_x\text{N}$ using the temperature dependent effective potential (TDEP) method [12] in combination with the symmetry imposed force constants (SIFC) approximation [13]. An approach which is called volume scaled simulations (VSS) [13] has been suggested based on the idea that the main contribution to the temperature variation of the elastic constants is caused by the thermal expansion of the material. Therefore, in this approximation the elastic constants at temperature of interest are calculated using static calculations at volume corresponding to that temperature which in its own turn is determined from the experimentally known or theoretically estimated thermal expansion coefficient of the material [13].

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Apparently, there is no accepted standard methodology yet for calculating the temperature variation of elastic constants of alloys. Therefore, benchmarking approximate methods is of enormous relevance in securing the quality of calculated data. In this study, we address this issue by performing highly accurate ab initio molecular dynamics simulations for one of the most common alloys used for coating of cutting tools, $\text{Ti}_{(1-x)}\text{Al}_x\text{N}$.

Metal machining is a complex process at high temperatures and high mechanical load. In general, elastic constants determine the response of the material at these conditions while the deformations are in the elastic regime. Linear elasticity is essential for determining forces acting and moving dislocations in materials, that is for understanding of plastic deformation [14]. Therefore, the knowledge of elastic constants supports the design of high-strength structural materials through phenomenological dislocation theories.

Elastic anisotropy in $\text{Ti}_{(1-x)}\text{Al}_x\text{N}$ has a particular relevance, because it affects the formation of the alloy microstructure upon spinodal decomposition, which results in an increase of the material's hardness [15,16]. This effect is called age hardening. Phase field simulations have confirmed the importance of the elastic energy term, in particular the elastic anisotropy in predicting the microstructure evolution during spinodal decomposition [17,18]. Experimental measurements of elastic properties of hard alloys synthesised in the form of thin films are challenging [19,20]. Therefore, numerous computational studies have been devoted to predict the elastic constants of $\text{Ti}_{(1-x)}\text{Al}_x\text{N}$ at different temperatures [13,21,22]. However, all elastic constants published so far for $\text{Ti}_{(1-x)}\text{Al}_x\text{N}$ includes different level of approximations in the calculations which were not benchmarked either against experiments or against accurate simulations.

In this study, we have carried out highly accurate calculations of the temperature dependence of the elastic constants of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ with ab-initio molecular dynamics simulations at 300, 600, 900, and 1500 K. The effect of alloying has been investigated through comparing the temperature variation of the elastic constants of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ with the ones of TiN. Moreover, we compare our results with those obtained by approximate VSS and SIFC-TDEP approaches [13,21–23]. Finally, we analyse the validity of the different approximate techniques: we evaluate if the accuracy of the results is justified by their computational costs. In addition, our data can be used as a reference to benchmark computational methods or to make comparison with on-going experimental studies on measuring temperature dependent elastic moduli of alloys for hard-coatings applications.

2. Theory and method

We calculate the second order stiffness tensor, C_{ij} , for B1 $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ using stress-strain relations which is a broadly accepted methodology for simulations of elastic properties of materials at zero temperature [24]. The stress-strain relation expressed with Voigt notation is written in Eq. (1), where the stress σ and strain ϵ are represented as vectors with six components.

$$\sigma_i = \sum_j C_{ij} \epsilon_j \quad (1)$$

Systems with cubic symmetry have only three independent elastic constants, C_{11} , C_{12} , and C_{44} , which are extracted by applying the deformation matrix,

$$\begin{pmatrix} 1+\eta & \eta/2 & 0 \\ \eta/2 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (2)$$

In Eq. (2), η defines the strain value, and the equations for elastic constants have the following form:

$$C_{11} = \frac{d\sigma_1}{d\eta}\bigg|_{\eta=0}, \quad C_{12} = \frac{d\sigma_2}{d\eta}\bigg|_{\eta=0}, \quad C_{44} = \frac{d\sigma_6}{d\eta}\bigg|_{\eta=0}. \quad (3)$$

To model chemical disorder in $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ we use the the supercell approach and distribute the alloy components at the sites of the supercells according to Special Quasi-Random Structures (SQS) method [25]. The SQS breaks the point symmetry of the simulated alloy whereas X-ray diffraction confirms cubic symmetry of $\text{Ti}_{(1-x)}\text{Al}_x\text{N}$ alloys [15]. This means that

$$C_{11} = C_{22} = C_{33}, \quad C_{12} = C_{23} = C_{13}, \quad C_{44} = C_{55} = C_{66} \quad (4)$$

in the real alloy, but in the supercell calculations the symmetry equations may not be fulfilled. To address this problem, the method of calculating the closest cubic projected elastic constants has been applied [22]. That is, one calculates the arithmetic average of the elastic constants obtained for the SQS;

$$\begin{aligned} \bar{C}_{11} &= \frac{C_{11} + C_{22} + C_{33}}{3}, \\ \bar{C}_{12} &= \frac{C_{12} + C_{13} + C_{23}}{3}, \\ \bar{C}_{44} &= \frac{C_{44} + C_{55} + C_{66}}{3}. \end{aligned} \quad (5)$$

Elastic constants at finite temperature are defined by the same linear stress-strain relationships, however one uses the averaged stress values obtained from the AIMD simulations.

3. Computational details

Parallel AIMD simulations were performed using an approach similar to the one proposed by Steneteg et al. [8]. To gain efficiency, we applied a two-steps procedure, starting our simulation runs with short low accuracy sequential AIMD runs. Then the high accuracy parallel AIMD simulations were initialized by taking uncorrelated samples from the initializing *low accuracy*, sequential AIMD simulations, see below for more details. The benefit of such an approach is the significant reduction of the computational walltime, though the consumption of computer resources is equal to one sequential simulation.

The simulations were carried out using the Vienna Ab initio Simulation Package (VASP), [26–29] with the projector augmented wave method [30]. The generalised gradient approximation in the form suggested by Perdew, Burke, and Ernzerhof [31] was used to calculate the exchange-correlation energy. We employed an energy cutoff of 600 eV, and a reciprocal space k -point sampling corresponding to a $(3 \times 3 \times 3)$ Monkhorst-Pack k -point grid. The second step high-accuracy molecular dynamics simulations were performed with a canonical ensemble at 300, 600, 900, and 1500 K using Nosé thermostat with default VASP settings and 0.5 fs as time-step. In the initializing first step *low accuracy* AIMD simulations, we used the Γ point sampling of the Brillouin zone. In the static density functional calculations for convergence testing the elastic constants of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ at $T = 0$ K were obtained as a function of the energy-cutoff and k -mesh density. We used $(4 \times 4 \times 4)$ SQS with 32 titanium, 32 aluminium, and 64 nitrogen atoms. The thermal expansion of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ was extracted from Ref. [13]. The AIMD simulations were carried out for the undistorted SQS and the supercells subjected to four deformations corresponding to η in Eq. (2) equal to -0.02 , -0.01 , 0.01 , and 0.02 .

For each simulation, the initial *low accuracy* runs included $\approx 20,000$ time-steps, from which 100 uncorrelated samples were extracted. We have selected these configurations such that the average and standard deviation of the potential and kinetic energy of these samples were equal to those of the all $\approx 20,000$ ones. 10 of the 100 samples were used as initial seeds for 10 parallel high accuracy AIMD simulations at the second step. These 10 simulations were run for ≈ 8000 time-steps altogether. The stresses were averaged over all these time-steps. Fig. 1 gives

Fig. 1. A representation of our parallel ab-initio molecular dynamics (AIMD) approach to calculate elastic constants $\bar{C}_{ij}$ at finite temperature. It shows the flow of the calculations in each of the five distortions with parameter η . The block MD 0 stands for the *low accuracy* AIMD simulations, which is followed by a sampling to select ten atomic configurations. The last block in each distortion shows the parallel performance of AIMD simulations started from these ten selected configurations.

a graphical representation of the flowchart of our parallel AIMD approach.

Before discussing the obtained results one should elucidate the amount of computational resources used in the simulations. In our approach we have performed calculations for five distortions with three orientations of the supercell at four temperatures. In each calculations we have performed low- and high-accuracy simulations. The simulations were running on a CRAY XC40 supercomputer. Each low-accuracy simulation has used approximately 13.800 core-hours, while in a high-accuracy simulation we have used 92.000 core-hours. In total, the highly accurate elastic constants of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ have been obtained with 6.348.000 core-hour computation. This is approximately 200 times more than what was used in case of applying SIFC-TDEP or VSS approximations [13].

4. Verification of numerical parameters used in simulations

To obtain highly accurate values of the elastic constants we first make sure that the simulations are fully converged with respect to the computational parameters. Since AIMD simulations are computationally demanding, we carry out these tests at $T = 0$ K using static DFT calculations and deriving the elastic constants from the stress-strain relations Eqs. (3) and (5) as explained above. We underline that the demands on numerical parameters used in AIMD calculations are in general lower than in static calculations because lattice vibrations often smear out peculiarities in the electronic structure which otherwise might require demanding parameters settings [11]. Thus, the convergence obtained in static tests ought to be sufficient for AIMD simulations.

The tests have been performed as follows. First, we kept the energy cutoff constant at 600 eV and varied the k-mesh sampling. Then we kept the $(3 \times 3 \times 3)$ k-mesh and varied the energy cutoff. The lattice parameter in all the test calculations was the same as for $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ at

300 K.

The results of these convergence tests are presented in Fig. 2. Fig. 2(a) shows the energy differences between undistorted ($\eta = 0.0$) and distorted supercells with $\eta = 0.01$ with varying energy cutoffs (left panel) and k-point densities (right panel). The required 1 meV/ion accuracy is achieved with $(3 \times 3 \times 3)$ k-point grid and the energy cutoff of ≈ 350 eV or with the $(2 \times 2 \times 2)$ k-point grid with the energy cutoff 600 eV. Any settings with values above these would therefore ensure the required accuracy in energy differences. Fig. 2(b) and (c) shows the variation of the pressure and stresses in the cell. These physical quantities are converged at a $(3 \times 3 \times 3)$ k-point grid and the energy cutoff of 500 eV or at $(2 \times 2 \times 2)$ k-point grid and the energy cutoff 600 eV. In Fig. 2(d) one sees the variation of the calculated elastic constants. The results show convergence at a $(3 \times 3 \times 3)$ k-point grid and energy cutoff of 400 eV. Thus, our analysis justifies the choice of the $(3 \times 3 \times 3)$ k-point grid and energy cutoff of 600 eV for AIMD simulations.

In Table 1, we have summarised calculated elastic constants of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ which have relevance for our later investigation at $T = 0$ K available in the literature and compare them with our results. In general, we observe very good agreement between the different calculations. Results reported in Ref. [13] deviate slightly from other calculations. The main reason for this could be that the $T = 0$ K data in Ref. [13] were not calculated explicitly, but rather obtained as an extrapolation from finite temperature simulations.

5. Results and discussion

Table 2 lists the obtained elastic constants of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ at the four simulation temperatures. Fig. 3 presents the temperature variation of $\bar{C}_{11}$, $\bar{C}_{12}$ and $\bar{C}_{44}$ obtained by different approaches. The results are shown with an alignment to their $T = 0$ K value, which allows us to compare the values obtained by different methods. In the figure the solid lines show our results. The elastic constants obtained by SIFC-TDEP calculations in Ref. [13] are drawn with dashed lines while the VSS results from the same work are presented with dash-dotted lines. The figure shows the expected softening of all three elastic constants with temperature. However, one sees significant differences in the results obtained by the different approaches. Note that the lattice parameter is the same in all the three methods. The difference between the full AIMD simulations and the VSS approximation at 1500 K for $\bar{C}_{11}$ is $\approx 17\%$, for $\bar{C}_{12}$ it is $\approx 19\%$, while for $\bar{C}_{44}$ one gets $\approx 15\%$. Moreover, VSS results in almost temperature independent values for $\bar{C}_{12}$ and $\bar{C}_{44}$. That is, the approximations employed in the VSS approach have significant effect on the predicted temperature variation of the elastic properties of the studied alloy. The use of the SIFC-TDEP method results in smaller differences with respect to the full AIMD calculations for all $\bar{C}_{ij}$. Still SIFC-TDEP tends to systematically overestimate the temperature softening of $\bar{C}_{12}$ and $\bar{C}_{44}$, while underestimating the softening of $\bar{C}_{11}$.

Fig. 4 displays the polycrystalline elastic moduli of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ calculated with the Hill averaging scheme [32,33]. It shows the bulk modulus (B_H), shear modulus (G_H), Young's modulus (E_H) and Pugh's ratio (B_H/G_H) based on the elastic constants obtained in this study and in Ref. [13]. For comparison, we show data for TiN using elastic constants from Ref. [8]. One sees similar softening trends of the elastic constants in both materials with increasing temperature. The values of all the elastic moduli are larger for TiN than $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$. Furthermore, one sees that the polycrystalline elastic constants calculated within the SIFC-TDEP approximation agree well with the ones obtained in this study. As the polycrystalline moduli are of very high relevance for practical applications, one concludes that the SIFC-TDEP approach provides sufficient accuracy to discuss elastic properties of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$.

For further characterization of mechanical properties, the simplistic, but widely accepted Pugh's ratio (B/G) is shown in Fig. 4(d). It predicts that $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ is more brittle than TiN while experiments show higher fracture toughness value for $\text{Ti}_{0.4}\text{Al}_{0.6}\text{N}$ than for TiN, see Ref. [19]. One

Fig. 2. Convergence of the total energy (a), pressure (b), stresses (c) and elastic constants (d) as a function of the plane wave energy cutoff (left figure) and Monkhorst-Pack k -mesh (right figure). In all the left figures the applied k -point mesh is $(3 \times 3 \times 3)$. In the right figures the applied energy cutoff is 600 eV.

notes that higher fracture toughness value indicates higher ductility and that the common failure of hard materials is brittle fracture [34]. This example illustrates that applications of phenomenologically derived models [4,35] may fail to predict hardness of hard coating alloys. The reason is that the above mentioned phenomenological models fail to capture the effects associated with microstructure of technological materials, like the age hardening and the solid solution hardening. Although the criteria have become popular based on selected successful demonstrations for ordered compounds, they should be used with great care for the design of hard coating alloys.

Fig. 5 shows an analysis of the elastic anisotropy in $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ in comparison with the elastic anisotropy calculated for TiN in Ref. [8]. Fig. 5(a) presents the directional distribution of the Young's modulus at 300, 900 and 1500 K. One sees that the absolute value of the modulus gets smaller with temperature, whereas its variation with the

crystallographic direction becomes larger. In addition, one observes the increase of the elastic anisotropy with temperature. We would like to note, that due to the temperature behavior of $\bar{C}_{ij}$ obtained by VSS, this approximation incorrectly predicts almost temperature independent anisotropy in $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$.

To have a closer look on the elastic anisotropy in these two materials we have calculated the distribution of Poisson ratio in three crystallographic planes, (100), (111) and (110). The results for $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ at 300 and 1500 K are shown in Fig. 5(b). For comparison the Poisson ratios of TiN are shown for the same temperatures in Fig. 5(c). Interestingly, in both materials one observes isotropic strain ratios in the (100) and (111) planes independently of the temperature, suggesting that the strength in these planes in response to a load perpendicular to the corresponding plane should be isotropic. In $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ the Poisson ratio is larger in the (100) plane than in the (111) unlike in TiN. One expects larger strength

Table 1Elastic constants of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ obtained at $T = 0$ K using different approaches and the applied numerical parameters.

Property	Ref. [22]		Ref. [13]	Ref. [23]	this study	
sym. averaging [22]	yes	yes	no	yes	no	yes
supercell size	$(4 \times 4 \times 3)$	$(4 \times 4 \times 4)$	$(4 \times 4 \times 4)$	$(4 \times 4 \times 3)$	$(4 \times 4 \times 4)$	$(4 \times 4 \times 4)$
energy cutoff (eV)	suff. conv.	suff. conv.	600	600	600	600
$\vec{k}$ points mesh	suff. conv.	suff. conv.	$(6 \times 6 \times 6)$	$(6 \times 6 \times 6)$	$(3 \times 3 \times 3)$	$(3 \times 3 \times 3)$
$\bar{C}_{11}$ (GPa)	447	454	430	447	461	466
$\bar{C}_{12}$ (GPa)	158	154	143	158	155	150
$\bar{C}_{44}$ (GPa)	203	202	189	203	197	200
A	1.40	1.34	1.31	1.41	1.29	1.27

Table 2Elastic constants of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ at four temperatures calculated in this study.

Temp. (K)	$\bar{C}_{11}$ (GPa)	$\bar{C}_{12}$ (GPa)	$\bar{C}_{44}$ (GPa)
300	423	153	202
600	396	150	195
900	362	146	188
1500	303	132	172

Fig. 3. Temperature variation of the elastic constants of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ calculated in this study. Results obtained in Ref. [13] by the symmetry imposed force constants approximation combined with the temperature dependent effective potential approach (SIFC-TDEP) and by volumed scaled simulations (VSS) are shown for comparison.

for smaller Poisson ratio. One sees also that the Poisson ratios for these two planes in $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ move apart from each other with temperature while the opposite trend is seen in TiN. The Poisson ratios in the (110) plane show significant anisotropy at high temperature in $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$, whereas, higher anisotropy occurs in TiN at room temperature. In this plane $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ is stiffer along the $[\bar{1}10]$ direction while TiN is stiffer perpendicular to this direction, along $[00\bar{1}]$. With increasing temperature $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ gets stiffer along $[\bar{1}10]$ direction and softer along the

$[001]$ direction. The same temperature effect is observed for TiN but it is less pronounced. While $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ becomes more anisotropic with temperature, TiN gets more isotropic.

For comparison, Fig. 5(d) shows the distribution of Poisson ratio in three crystallographic planes, (100), (111) and (110) calculated at 0 K with increasing Al content. The $T = 0$ K elastic constants are taken from Ref. [21]. One sees that the material is almost isotropic for $x = 0.25$ and becomes highly anisotropic with $x = 0.75$ Al content. This agrees with the observation in Ref. [21]. Interestingly, one observes that increasing Al content affects the material's elastic anisotropy to the similar degree as increasing temperature.

Fig. 4. Temperature variation of the Hill averaged polycrystalline elastic moduli, such as bulk (B_H), shear (G_H), Young's (E_H) and Pugh's ratio (B_H/G_H) of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ and TiN. Solid line shows the results derived in this study, dashed line shows the results obtained by SIFC-TEDP method in Ref. [13] and the dotted line presents the results for TiN obtained by AIMD in Ref. [8].

Fig. 5. Directional elastic anisotropy of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ and TiN at elevated temperatures. (a) shows the value of the directional Young's modulus in $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$. (b) and (c) display the directional variation of Poisson ratio in $[100]$, $[111]$ and $[110]$ planes for $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ and TiN , respectively. For comparison, (d) shows the variation of the distribution of Poisson ratio in $[100]$, $[111]$ and $[110]$ planes with varying Al content at T=0 K using the elastic constants from Ref. [21].

6. Conclusions

In summary we have calculated highly accurate temperature dependent elastic constants of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ using parallel AIMD simulations and compared our results with those obtained for TiN in Ref. [8]. The derived polycrystalline elastic constants have shown the expected softening with increased temperature in both materials. From the analyses of the directional Young's moduli and Poisson ratios calculated on the (100), (110) and (111) crystallographic planes we have concluded that the elastic anisotropy of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ increases with temperature unlike in TiN. Moreover, we compared our results with those obtained by the methods which introduce different additional approximations for the treatment of finite temperature effects on elastic moduli and concluded that the symmetry imposed force constants approximation combined with the temperature dependent effective potential method (SIFC-TDEP) predicted accurate elastic constants and polycrystalline elastic moduli of $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$. The comparison of the used computational resources has shown that SIFC-TDEP approach is approximately 200 times more efficient that justifies its use for simulations of hard coating alloys.

CRediT authorship contribution statement

Johan Tidholm: Investigation, Formal analysis, Visualization, Writing – original draft. **Ferenc Tasnádi:** Conceptualization, Validation, Formal analysis, Writing – review & editing, Supervision. **Igor A. Abrikosov:** Conceptualization, Formal analysis, Writing – review & editing, Supervision.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary material

Supplementary material associated with this article can be found, in the online version, at doi:[10.1016/j.tsf.2021.138872](https://doi.org/10.1016/j.tsf.2021.138872)

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