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Ab initio calculations of elastic properties of Ni_3Al and TiAl under pressure*

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The structural parameters and the elastic stiffness coeffcients of Ni_3Al and TiAl under a pressure P were computed by the *ab initio* pseudopotential method with the plane-wave basis set and the generalized gradient approximtion (GGA). The pressure dependence of the elastic constants is an important characteristics for both Ni_3Al and TiAl as these materials are frequently subject to varying pressures during processing. The bulk modulus was also calculated. Stress–strain relationships were used to obtain the elastic constants. The results are in good agreement with the available experimental data.

Key words: *ab initio calculations; density functional calculations*

1. Introduction

In recent years, *ab initio* computations have become one of important tools of modern computational materials science. In the present work, first principles calculations were undertaken for Ni_3Al and TiAl under a pressure P. Ni_3Al compound is known to crystallize in a cubic lattice of Cu_3Au structure type with the space group $Pm\bar{3}m$, while TiAl crystallizes in a tetragonal lattice of AuCu structure type with the space group $P4/mmm$.

2. Computations

For the computations of the crystal structures, ultrasoft pseudopotentials on the assumption of the Gradient Generalized Approximation (GGA) were adopted. The CASTEP [1] program was employed and the computations were carried out at the

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ICM of Warsaw University. CASTEP is a DFT pseudopotential total-energy code employing special point integration over the Brillouin zone and a plane-wave basis set for the expansion of the wave functions. The Monkhorst-Pack scheme was used to sample the Brillouin zone. The calculations were considered converged when forces acting on the atoms were less then 0.01 eV/A and the residual bulk stress was smaller than 0.02 GPa. The complete elastic constant tensor from computation of the stresses generated by small deformations of the equilibrium primitive cell [2, 3] was determined. The elastic stiffness tensor $\mathbf{C}$ relates the stress tensor $\boldsymbol{\sigma}$ and the strain $\boldsymbol{\varepsilon}$ by Hooke's law,

$$\sigma_{ij} = C_{ijkl}\,\varepsilon_{kl} \qquad (i,j,k,l = x,y,z) \tag{1}$$

Since the stress and strain tensors are symmetric, the most general elastic stiffness tensor has only 21 non-zero independent components. For cubic crystals, they are reduced to three independent components, $C_{11} \equiv C_{xxxx}$, $C_{12} \equiv C_{xxyy}$, $C_{44} \equiv C_{yzyz}$, (in the Voigt notation). For tetragonal crystals, they are reduced to 6 components.

3. Results

The intermetallic phases, TiAl and Ni_3Al, have been studied by *ab initio* calculations under an applied pressure P. The results for zero-pressure are summarized in Tables 1 and 2 showing the lattice parameters, elastic constants and C_{ij} values calculated *ab initio*, in comparison with experimental data [4–6].

Table 1. Zero-pressure lattice parameters and elastic constants for the Ni_3Al ground-state structure

Method	a [Å]	C_{11} [GPa]	C_{44} [GPa]	C_{12} [GPa]
Ab initio	3.588	230	123	139
Experimental	3.572	230	131	150

Table 2. Zero-pressure lattice parameters and elastic constants for the TiAl ground-state structure

Method	a [Å]	c [Å]	C_{11}[GPa]	C_{33}[GPa]	C_{44}[GPa]	C_{66}[GPa]	C_{12}[GPa]	C_{13}[GPa]
Ab initio	3.989	4.034	170	177	113	73	79	78
Experimental	3.99	4.07	183	178	105	78	74	74

The results of computations under applied pressure P are shown in Figs. 1 and 2 where elastic stiffness C_{ij} is plotted against P.

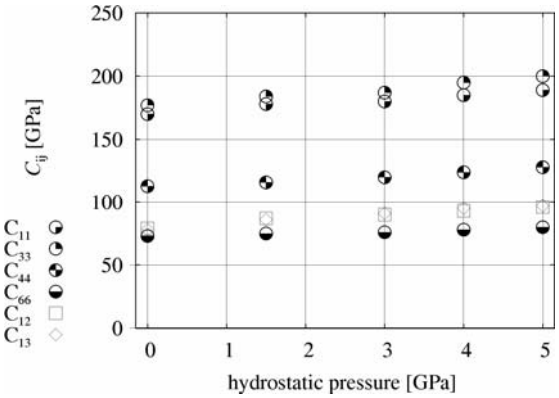

Fig. 1. Elastic stiffness coefficients of TiAl under hydrostatic pressure

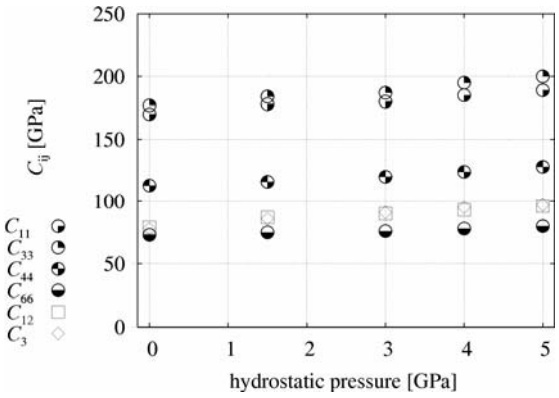

Fig. 2. Elastic stiffness coefficients of Ni_3Al under hydrostatic pressure

These elastic stiffness coefficients satisfy the generalized elastic stability criteria for cubic (Eq. 2) and tetragonal (Eq. 3) crystals under hydrostatic pressure

$$C_{43} > 0, C_{11} > |C_{12}|, C_{11} + 2C_{12} > 0 \tag{2}$$

$$\begin{gathered} C_{11} - C_{12} > 0, \qquad \frac{1}{2}(C_{11} - C_{12})C_{33} - C_{12}^2 > 0 \\ C_{11} + C_{12} + C_{33} + \sqrt{(C_{11} + C_{12} - C_{33})^2 + 8C_{13}^2} > 0 \\ C_{44} > 0, C_{66} > 0 \end{gathered} \tag{3}$$

Ab initio computations have been also used to calculate the bulk modulus of the phases *B*, being equal to 109 GPa for TiAl, and 203 for Ni_3Al. Again this is close to the literature value of 108 GPa [5] for TiAl, and 208 GPa [5] for Ni_3Al.

4. Conclusions

Results of *ab initio* calculations for zero pressure are in good agreement with avaiable experimental data (cell constants, elastic constants, bulk moduli). It should be noted that the $C_{ij}(P)$ for Ni_3Al increase linearly with increasing pressure.

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References

[1] SEGALL M.D., LINDAN P.L.D., PROBERT M.J., PICKARD C.J., HASNIP P.J., CLARK S.J., PAYNE M.C., *First-principles simulation: ideas, illustrations and the CASTEP code*, J. Phys.: Cond. Matt. 14 (2002), 2717.

[2] KARK B.B. I, STIXRUDE L., CLARK S.J., WARREN M.C., ACKLAND G.J., CRAIN J., Am. Mineral., 82 (1997), 51

[3] WENTZCOVITCH R.M., ROSS N.L., PRIECE G.D., Phys. Earth Planet. Int., 90 (1995), 101.

[4] ICDD 09-0097, J. Met., 9 (1957), 865.

[5] SIMMONS G., WANG H., Single C*rystal Elastic Constans and Calculated Aggregate Properties: A Handbook*, MIT Press, Cambridge, 1971.

[6] *Smithells Metals Reference Book*, 6th Ed., E.A. Brandes (Ed.), Butterworths, London, (1983)

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