6.1 First-Principles Investigation of the Influence of Alloying Elements on the Elastic and Mechanical Properties of Tungsten — G. D. Samolyuk, Y. N. Osetskiy, and R. E. Stoller (Oak Ridge National Laboratory)

OBJECTIVE

The objective of this research is to support possible approaches to the design of ductile tungsten alloys through the use of relevant *ab initio* electronic structure calculations.

SUMMARY

The properties of ½<111> screw dislocations in $W_{1-x}Tm_x$ alloys with different transition metal, Tm, concentrations within the local density approximation of density functional theory was investigated. The electronic structure of alloys was described within the virtual crystal approximation. It was demonstrated that alloying of W with transition metals from group VIII modifies the properties of screw dislocation similar to the effect of alloying with Re. Specifically, the alloying changes the dislocation core from symmetric to asymmetric and reduces the value of the Peierls barrier and Peierls stress. These modifications are caused by filling of d-electron states of W.

PROGRESS AND STATUS

Introduction

Alloys of W with Re have been studied extensively using both experiment [1, 2] and theory [3, 4, 5]. Adding Re has the effect of ductility improvement of the tungsten. In [5] it was demonstrated using first principles calculations that addition of Re to tungsten modifies the symmetry properties of ½<111> screw dislocations and reduces the value of the Peierls barrier. In the present research we investigate the properties of screw dislocations in binary $W_{1-x}Tm_x$ using first-principles electronic structure calculations for a set of transition metals (Tm). This result will be used in a future search for alloying elements causing changes in tungsten alloys properties similar to the effects of Re.

Formalism

We calculated the electronic structure within the local density approximation of density functional theory (DFT) using the quantum espresso package [6]. The plane wave energy cut off at 42 Ry allows accuracy 0.2 mRy/atom. The alloying was modeled using the virtual crystal approximation (VCA). As a realization of VCA for the pseudo potential method we used the scheme proposed in Ref. [7]. A periodic quadrupole arrangement of ½<111> screw dislocation was used to describe the core structure and Peierls barrier. Two dislocations with opposite Burgers vectors were placed in a super cell containing 135 atoms with lattice vectors $\boldsymbol{b}_1=(9\boldsymbol{u}_1+5\boldsymbol{u}_2+\boldsymbol{u}_3)/2$, $\boldsymbol{b}_2=5\boldsymbol{u}_2$ and $\boldsymbol{b}_3=\boldsymbol{u}_3$, where vectors $\boldsymbol{u}_1$=<112>, $\boldsymbol{u}_2$=<110> and $\boldsymbol{u}_3$=<111>/2. The BZ summations were carried out over a 1x2x8 BZ grid with Gaussian boarding of 0.02 Ry. It was demonstrated that summation over 1x1x3 BZ grid used in our previous calculation in not accurate enough. The Peierls barrier in $W_{1-x}Tm_x$ was obtained by moving a ½<111> dislocation from easy to hard core configurations.

RESULTS

The applicability of the virtual crystal approximation to $W_{1-x}Re_x$ binary alloys was verified in our previous research, see [9]. Also it was demonstrated that the so-called rigid band approximation

can be applied. Thus, all dilute tungsten based alloys with the same number of electrons per atom (*e*/*a*) have the same elastic constants. The concentration of different alloying elements which give the same (*e*/*a*) value can be calculated through the simple expression

$$x = \frac{(e/a)}{Z - Z_W}, \tag{1}$$

where Z is the number of valence electrons of the alloying transition metal atom and Z_W of tungsten. As it was demonstrated in our previous reports [9], the d band filling by addition of electrons from the VIII group transition metal, the lattice parameter decreases and elastic anisotropy $A=C_{44}/C'$ increase [9]. The obtained result agrees with experiment [10]. Also the C' and A values demonstrate very close dependence on concentration if they are plotted as a function of (*e*/*a*), the number of electrons per atom. This similarity supports conclusion that the main effect of alloying W with transition metals with larger number of *d* electrons is related to *d* band filling.

The calculated structure of the easy core configuration of a 1/2<111> dislocation is shown on Fig. 1 for pure W, $W_{0.75}Re_{0.25}$ and $W_{0.88}Fe_{0.12}$, where concentrations of transition metals were chosen to give the same (*e*/*a*) value. The circles on Fig. 1 represent W atoms looking in the <111> direction and the structure of dislocation is illustrated by differential displacement maps [11]. It should be mentioned that for tungsten alloys with other Tm with the same (*e*/*a*) value the core configurations are the same as for Re and Fe alloys but are not shown here. As was demonstrated in [5] for W a symmetric core is obtained, i.e. the dislocation expands equally along the six <112> directions.

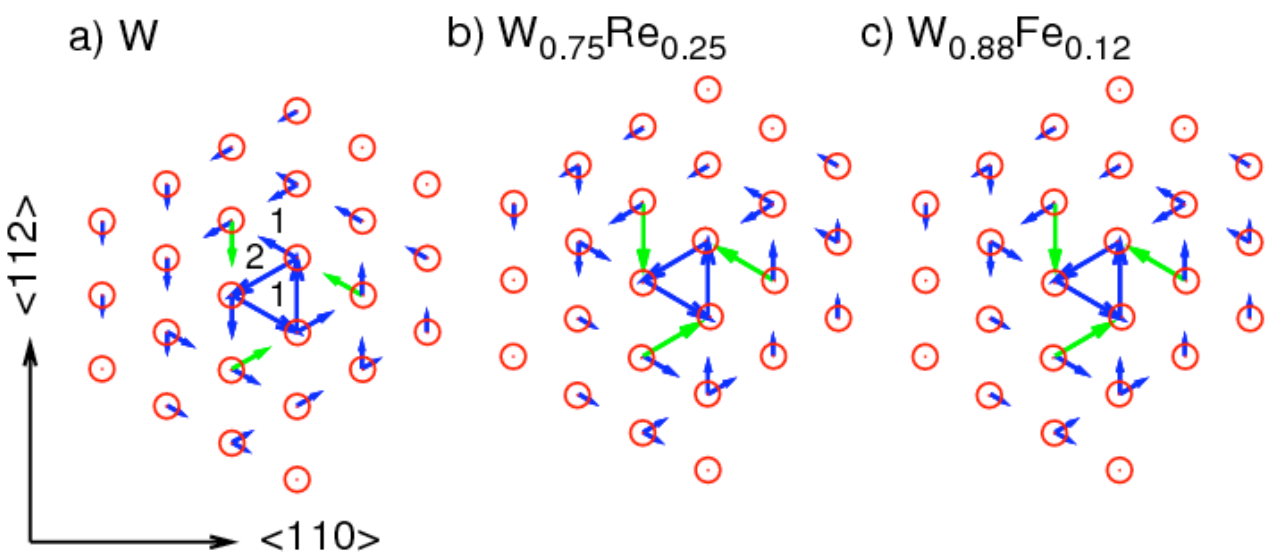

Figure 1. The easy core dislocation structure in $W_{1-x}Tm_x$ calculated in VCA.

Alloying with Re or any other Tm with the same value of (*e*/*a*) leads to change from a symmetric core structure to an asymmetric structure. It should be mentioned that increase of BZ grid size modifies Tm concentration at which the symmetry core change can bi visualized to larger concentrations. As was mentioned in Ref [5], the transition from symmetric to asymmetric cores changes the dislocation slip plane. The symmetric core dislocations move uniformly on {110} planes; asymmetric ones move in a zigzag manner [12] and the slip plane changes to {112}.

Along with the change of core symmetry the value of the Peierls barrier changes, see Fig. 2. As can be seen, alloying with Re, and Tm from VIII group with concentration which corresponds to

(e/a)=6.05 reduces the barrier by ~25 %, whereas Zr increases the barrier and makes the tungsten alloy more brittle.

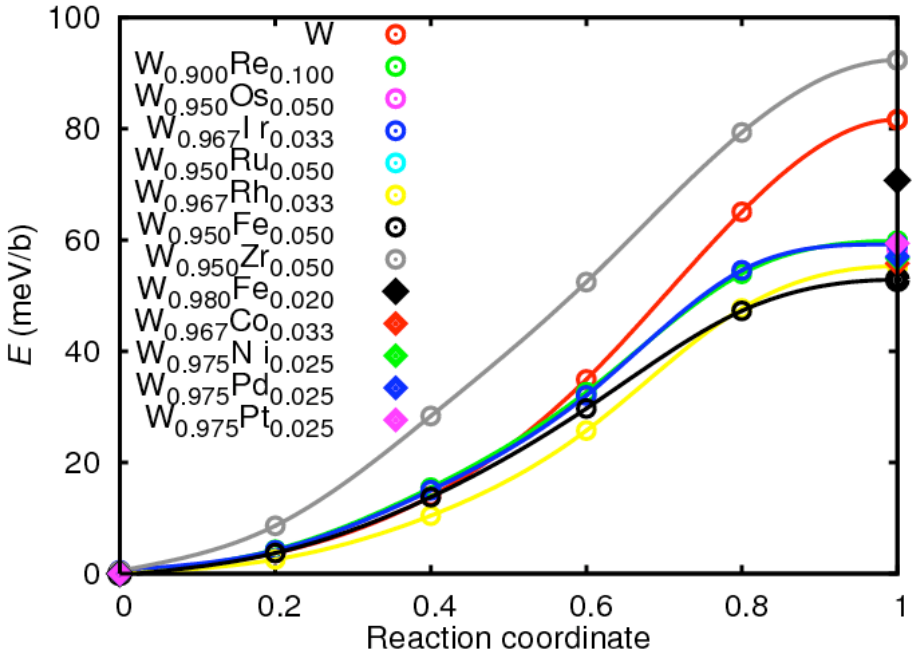

Figure 2. Calculated Peierls barrier in $W_{1-x}Tm_x$.

The concentration of Tm in these calculations was chosen thus that it keeps the same value (e/a). However the limit of solubility of Fe in W is < 2 %. The result for modification of Peierls barrier for 2 % Fe is shown by black diamond on Fig. 2 and equals ~ 10%. Although Peierls barrier is very important property of dislocation it's not directly determine value of Peierls stress, the stress should be applied to crystal to move dislocation from one easy core configuration to another one. The value of Peierls stress can be calculated directly by applying strain to modeling cell until the dislocation moves. The strain was applied by modification of lattice vector $\boldsymbol{b}_1=9/2\boldsymbol{u}_1+5/2\boldsymbol{u}_2+(1/2+\xi)\boldsymbol{u}_3$. On the Fig. 3 the dependence of modeling cell energy as a function of strain ξ is presented.

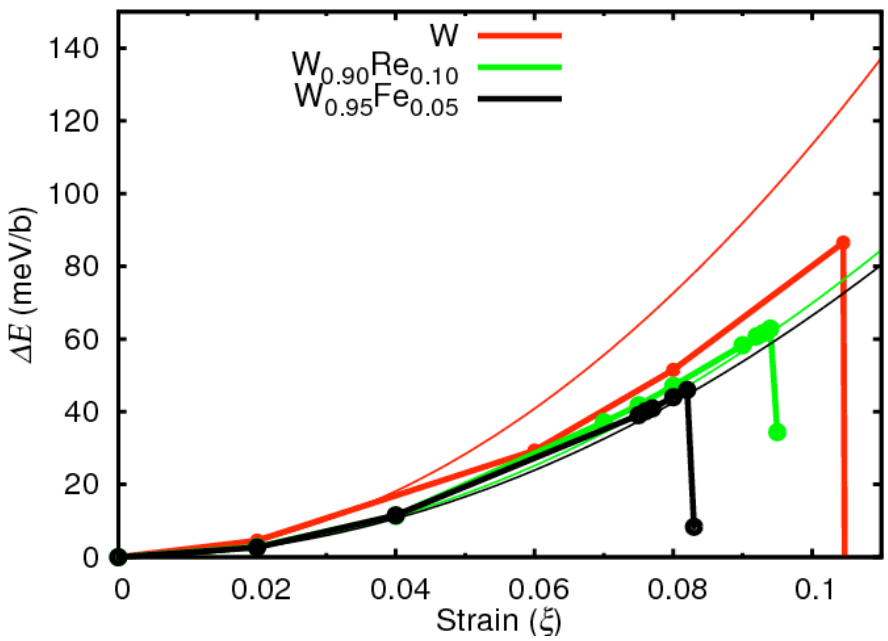

Figure 3. Energy of modeling cell as a function of strain *ξ*.

The drop in the total energy corresponds to dislocation glide and obtained value of the stress corresponds to Peierls stress. Thus the alloying reduces Peierls stress from 1.71 GPa to 1.37 GPa for 10 % Re and to 1.1 GPa for 5% of Fe. The correlation between Peierls barrier as a function of reaction coordinate (blue) and energy of the modeling cell as a function of strain (red) is illustrated on Fig. 4.

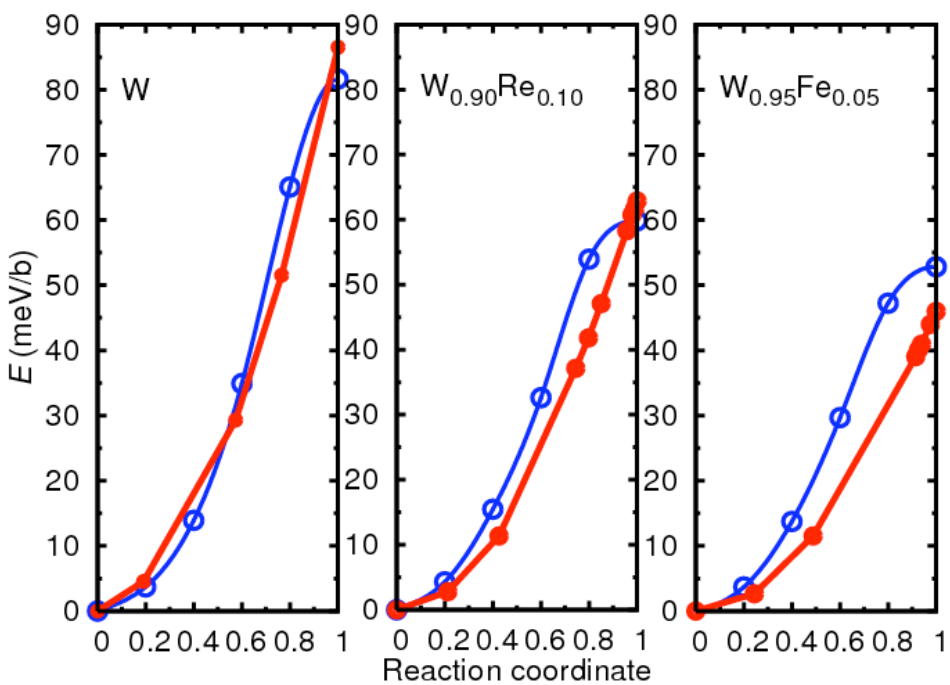

Figure 4. Energy of modeling cell as a function of strain *ξ* (red) and Peierls barrier (blue).

The energy as a function of strain is rescaled thus that zero corresponds to zero strain and one to Peierls stress. As it can be seen the value of total energy of cell at Peierls stress is qualitative agreement with value of Peierls barrier and modification of Peierls barrier can be used as a screening to gauge ductility.

Thus the alloying tungsten with any transition metal from VIIA and VIIIA groups leads to similar modifications of dislocation core structure and reduction of the Peierls barrier and Peierls stress and possible ductilizing effect.

References

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