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Calculation E.A.M potentials for tungsten trioxide WO_3

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Abstract

The pair potential model was used to determine the EAM potential of tungsten trioxide. The mixed potential was initially calculated as a linear combination of the potentials of the interacting elements through embedding function, electron density function and energy. For ordered phases, the results of a composition of the potentials at the stoichiometric WO_3 concentration do not make possible to obtain the lattice constants of any phase, some transformations have been made to the mixed potential by the adjustment of the variable r for each term of the first and second members of the equation defining the mixed potential. Thus, according to the fixed parameter (a, b), the lattice parameters were found for the trioxide of tungsten (WO_3) phase in agreement with the theoretical lattice constants and was used to validate the E.A.M model in the case of an ordered phase under stoichiometric conditions.

Keywords: Embedded atom method (EAM), ordered phase, stoichiometry, trioxide of tungsten, WO_3 potential, lattice constant.

Introduction

In recent years, a number of promising nanometallic compounds are being studied for industrial applications[1-4].

Alloys are being studied because of their low density, these alloys have been considered attractive candidates for applications in advanced aerospace engine components and have potential for enhanced performance. The embedded atom method (EAM)[5,6] is generally used for this type of atomistic simulation.

The EAM potential for a system is generally set up on the basis of that for its constituent elements. Different functions of ρ,ϕ, and F have been proposed for various elements according to their structures and properties. The function proposed by Pasianot and Savino[5-9,14] is selected to describe EAM potential of materials with hcp structure, since it takes the contribution of internal relaxation to the elastic constants due to the existence of two atoms per primitive lattice cell in the hcp structure[8], which are termed inner elastic constant. The potential function proposed by Voter[9,10] is selected for fcc structure.

The effect of oxygen concentration in the development of the potential of tungsten oxide has an interest in predicting the properties of tungsten oxides for the development of catalysts, sensors and materials for aeronautics[11,20]. The purpose of this paper is to calculate the E.A.M potential of trioxide of tungsten (WO_3).

Model

Within the frame of the EAM theory[6], the total internal energy E_{tot} of any atomic structure, is described as the sum of two terms, an embedded atom term F which depends on the local electron density ρ, and a pair-potential term ϕ which depends purely on interatomic distance r.

$$E_{total} = \sum_{\alpha=A,B} F_\alpha(\rho_\alpha) + \frac{1}{2}\sum_{\alpha=A,B}\phi_\alpha(r) \quad (1)$$

Where, F_α, ρ_α , Φ_α are effective embedding function, effective charge density, effective pair-wise energy for the effective atom at the type α site respectively.

The Foiles 'scheme[22,23] is used to obtain F(ρ) over the necessary range.

From

$$E = F(\rho) + \frac{1}{2}\sum_m \phi(r^m) \quad (2)$$

$$\rho = \sum_m f(r^m) \quad (3)$$

Where E is the energy per atom, and r^m the *m*th neighbor distance to some particular atom.

In order to apply the EAM, the f, ϕ and F must be given from equation (2)

The average energy of each atom is

$$E_l = \sum_{\alpha=A,B} C_\alpha E_\alpha \quad (4)$$

Results and discussion

Mixed E.A.M potential of stoichiometric tungsten trioxide: We have chosen the resulting potential in the case of stoichiometric composition taking in account the interaction potential of the oxygen (O) and tungsten (W):

$$\phi^{wo}(a+bx) = 0.25\phi^{ww}(c+dx) + 0.75\phi^{oo}(e+fx)$$

r = a + b*x= c + dx= e + fx where 0<x<1

This form does not allow us to simulate several crystallographic phases produced by this compound. However, to include the relaxations (different atomic positions) that can lead us to a crystallographic variety, a transformation of the value of the interatomic distance is necessary.

Mathematically this would lead to a framing of the value of r by the parameters

a <r <a + b

However, a and b are not known and represent only parameters to be fixed. On the other hand we have here, rather framed the parameters to be fixed. The value a represents a normalization constant that we will calculate later; However, we have set an arbitrary constant for all mixed potential curves.

Table-1: E.A.M. mixed potential parameters.

Parameters	valeurs. 10^{-1}nm	
A	0.25	
A	1.000	3.0
B	7.65	7.60
C	1.000	3.000
D	7.65	7.60
E	1.000	3.0
f	7.65	7.60
aa	1.200 ev	1.200ev

Giving the type of compound W_xO_y, composed of crystallographic structures which would have a stoichiometric composition under the variable influence of the concentration of each constituent element; we added for each of the terms of the left members of our mixed potential, the value of "x" responsible for the concentration then influencing the composition of the final composite.

To translate this mixed potential according to the crystallographic form, we used the crystallographic quantities of the cubic WO3 (monoclinic) structure.

Table-2: E.A.M parameters for cubic WO3 (monoclinic) structure.

a	7.30
b	7.60
c	7.60

For Oxygen we chose the inter-atomic potential given by Xia Wang Zhou[9,10].

Several potentials of tungsten for both the centered cubic structure and its angular electronic behavior due to the valence layer d; are proposed, namely the potentials of Morse, as well as Finnis Sinclair[3]. In this work, the analytical form of the tungsten potential is defined by Mendeleev and Ackland and al[5], whose fixing conditions are defined by M.C. Maranica.

In order to include the relaxations, a transformation of the value of the interatomic distance is necessary; We have inserted the value of "x" between 0 and 1 acting on the interatomic distance of the mixed potential.

Mixed electron density of WO_3
$$\rho^{wo3}(r) = 0.25\rho^{ww}(r) + 0.75\rho^{oo}(r)$$

Total energy of WO3
$$E^{wo3}(r) = 0.25E^{ww}(r) + 0.75E^{oo}(r)$$

E^{ww}et$E^{oo}$are total energy of tungsten ang oxygen respectively

Embedding Function of WO_3: The calculated embedding function can be deduced using the following equation:

$$F(\rho) = E^{wo3}(r) - \frac{1}{2}\phi^{wo3}(r)$$

At the stoichiometric composition the embedding function ca be written:

$$F^{wo3}(r) = 0.25F^{ww}(r) + 0.75F^{oo}(r)$$

Table-3: Physical parameters for WO_3 structures.

	Lattice	Constant	
Structure	Monoclinique-WO3	Hexagonal - WO3	Cubic WO3
Fitting Parameters	5.25	7.30	3.82
a	6.0	4.6	2.0
b	3.60	7.60	5.20
c	5.000	2.000	2.000
d	7.60	7.60	4.60
e	5.0	2.0	2.0
f	4.60	5.60	5.60
aa	1.200	1.200	1.200

Although we have already taken a step towards the different crystallographic structures, we still cannot explain the influence of the concentration of the elements involved because hitherto the concentration is fixed at the stoichiometry of 0.25% tungsten 0.75%.

To better manipulate the mixed potential, through all these ordered forms and phases and to predict disordered phases (if possible); Giving the type of compound WxOy, composed of crystallographic structures which would have a stoichiometric or non-stoichiometric composition under the variable influence of the concentration of each constituent element; We added for each of the terms of the left members of our mixed potential, the value of "x" responsible for the concentration then influencing the composition of the final composite.

Thus the study carried out for a few phases allowed us to plot the potentials for fixed torque values as indicated in the figures.

The E.A.M function of WO_3 are presented in the Figure-1, 2 and 3, the results show a good agreement with literature results. The non linearity of these function can be attributed to the many body effects.

The potential becomes more repulsive as the density increases. The E.A.M potentials for tungsten is found in qualitative agreement with DFT calculation.

Conclusion

The pair potential model was used to determine the EAM potential of tungsten trioxide. The individual potentials of the interacting elements were firstly determined using literature data and validate through the calculated lattice constant. For ordered phases at the stoichiometric WO_3 concentration, some transformations have been made to the mixed potential. Thus, according to the fixed parameter (a, b), the lattice constants were found for each trioxide of tungsten (WO_3) phase in agreement with the theoretical lattice constants and was used to validate the E.A.M model in the case of an ordered phase under stoichiometrical conditions.

The E.A.M potential obtained is used to predict the transitions properties of any structure of WO_3. EAM potentials for WO3 were found to be in agreement with DFT calculations.

To predict the disordered phases in the case of the non-stoichiometric composition; a new modification must be made.

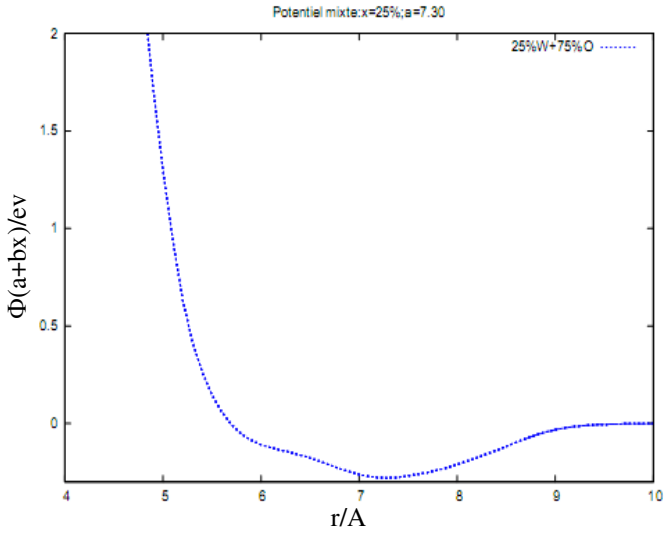

Figure-1: Pair potential for hexagonal WO3 at stoichiometric composition.

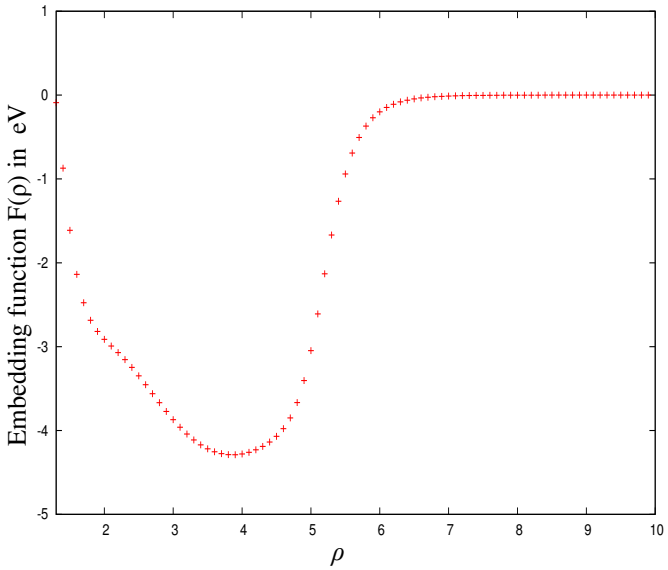

Figure-2: Embedding function of hexagonal trioxide tungsten at stœchiometric composition.

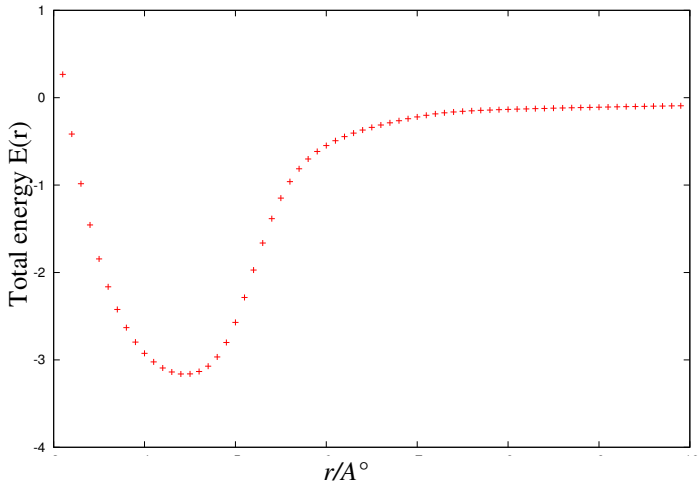

Figure-3: Total energy of hexagonal trioxide tungsten at stœchiometric composition.

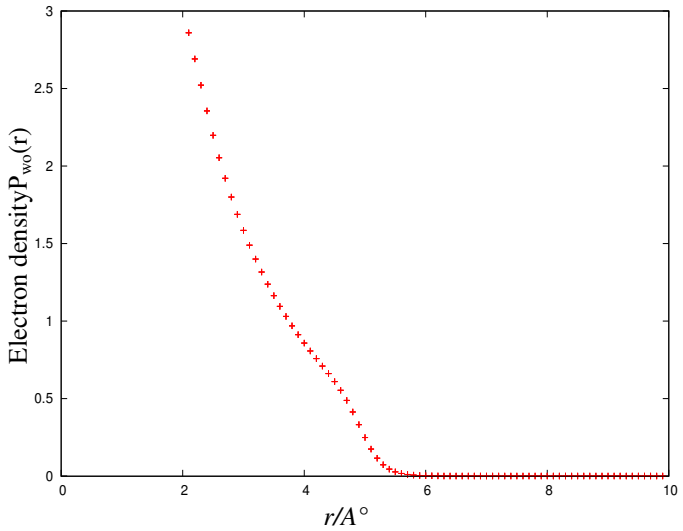

Figure-4: Electron density of hexagonal trioxide tungsten at stœchiometric composition.

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