



involves an stoichiometric inhomogeneity in the extreme limit of the existence of compounds (C_2) with interior stoichiometries ($C_{1.5}$, $C_{1.8}$, $C_{2.2}$, $C_{2.5}$, $C_{2.8}$).

Under these conditions, the energy minimization achieved 11% underestimation of the surface energy.

Understandably, a number of phenomena can be explained by this effect. In particular, there were many attempts that used the extensive and successful

models of the formation energies of point defects to calculate the orientation of the first principle self-consistent electron structure theory and defect pairs and arrays in

understanding of various inhomogeneities in the dependence of characteristics on formation energies on the chemical potentials and Fermi levels versus considered

defects. As a result, these models have serious shortcomings, which the first principle self-consistent electron structure theory and defect pairs and arrays in

2. Method of Calculating Circumference

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10. *What is the primary purpose of the following statement?*

$\tilde{f}_k^{\text{eq}}(t)$) can be rewritten as

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* 8. *Is it true that the point*

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0.800 0.100 0.000

10.1007/s00332-017-9170-2

Figure 10. A comparison of the results of the two methods for the same data set.

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Figure 1. A schematic diagram of the experimental setup. The light source (labeled 1) is a pulsed Nd:YAG laser operating at 532 nm. The beam passes through a lens (labeled 2) and is focused onto a sample (labeled 3). The sample is a thin film of polyimide deposited on a substrate. The beam is reflected by the sample and passes through a lens (labeled 4) and a polarizer (labeled 5). The polarized light is detected by a photodiode (labeled 6).

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Figure 1. A grayscale image of a scene containing a white car, a black car, and a white van.

$$\Delta E = \gamma_1^2 + \gamma_2^2 + \dots + \gamma_n^2 - \Delta H(CuInSe_3) \quad (5)$$

formation of binaries

from the elemental sulfur having binding values that will cause

(e.g., In_2Se_3 and Cu_2Se).

formed until $\Delta E = 0$ is met. This defines the defect transition criteria that can be used to predict the formation of new phases. It is interesting to note that this will

not always be at another charge, i.e., $+1, +2, \dots$.

Fig. 1.

We calculate the defect energy ΔE in eV, V_{def} in cm^{-3} , and the defect density N_{def}

$y = d/a = 1.108$ where d is the distance between the centers of two adjacent atoms in a face-centered cubic lattice at the center of a 3×3 array of vectors ($1/2, 1/2, 1/2$) in units of $a/2$, where $a = 5.798 \text{ \AA}$, as de-

scribed by the following equation:

$y = \sqrt{3}/4 = 0.433$ where $y = d/a$ and $a = 5.798 \text{ \AA}$.

The calculated defect energy ΔE is plotted in Fig. 1 as a function of the defect density V_{def} for various values of the defect radius r .

It is evident from Fig. 1 that the defect energy ΔE increases with increasing defect density V_{def} and decreases with increasing defect radius r .

The calculated defect energy ΔE is plotted in Fig. 2 as a function of the defect radius r for various values of the defect density V_{def} .

It is evident from Fig. 2 that the defect energy ΔE increases with increasing defect radius r and decreases with increasing defect density V_{def} .

The calculated defect energy ΔE is plotted in Fig. 3 as a function of the defect radius r for various values of the defect density V_{def} .

It is evident from Fig. 3 that the defect energy ΔE increases with increasing defect radius r and decreases with increasing defect density V_{def} .

The calculated defect energy ΔE is plotted in Fig. 4 as a function of the defect radius r for various values of the defect density V_{def} .

It is evident from Fig. 4 that the defect energy ΔE increases with increasing defect radius r and decreases with increasing defect density V_{def} .

The calculated defect energy ΔE is plotted in Fig. 5 as a function of the defect radius r for various values of the defect density V_{def} .

It is evident from Fig. 5 that the defect energy ΔE increases with increasing defect radius r and decreases with increasing defect density V_{def} .

The calculated defect energy ΔE is plotted in Fig. 6 as a function of the defect radius r for various values of the defect density V_{def} .

It is evident from Fig. 6 that the defect energy ΔE increases with increasing defect radius r and decreases with increasing defect density V_{def} .

The calculated defect energy ΔE is plotted in Fig. 7 as a function of the defect radius r for various values of the defect density V_{def} .

It is evident from Fig. 7 that the defect energy ΔE increases with increasing defect radius r and decreases with increasing defect density V_{def} .

The calculated defect energy ΔE is plotted in Fig. 8 as a function of the defect radius r for various values of the defect density V_{def} .

It is evident from Fig. 8 that the defect energy ΔE increases with increasing defect radius r and decreases with increasing defect density V_{def} .

The calculated defect energy ΔE is plotted in Fig. 9 as a function of the defect radius r for various values of the defect density V_{def} .

It is evident from Fig. 9 that the defect energy ΔE increases with increasing defect radius r and decreases with increasing defect density V_{def} .

The calculated defect energy ΔE is plotted in Fig. 10 as a function of the defect radius r for various values of the defect density V_{def} .

It is evident from Fig. 10 that the defect energy ΔE increases with increasing defect radius r and decreases with increasing defect density V_{def} .

Table 1. Defect formation energies $\Delta E(\text{eV})$ in Wg_2Te_3 and defect transition levels.

$$^{i+m})\mathfrak{Se}_{2n} + \beta m(\mathbb{C}\mathbf{u}) = \Delta H_f(n, m), \quad (7)$$

and nuclear energy (1.8% of total electricity generation).

where $m = 1, 2, 3, \dots$ and $n = 2, 4, 5, \dots$

The analysis shows that the interaction and driving energies ΔH_f and ΔG_f for the direct In^{2+} array ($2V_{\text{In}} + \text{In}^{2+}$) is about 2.6 eV, which is less than ΔH_f of the In^{2+} array at point A. The standard enthalpy of formation, $\Delta H_f(\text{In}^0) = -45 \text{ eV}$, at point A in Fig. 1.

Thus, spontaneous formation of stable

array could be as low as -6.1 eV at point B.



For isolated interacting ($2V_{Cu}^- + \hat{In}_{Cu}^{e+}$) pair, we find that the pairing pushes up the down In_{Cu}^- levels to positions much closer to the conduction band minimum.



References

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