khadija paper on α-U

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Abstract

1. Introduction

2. Computational Details

The Large-scale Molecular Massively Parallel Simulator (LAMMPS) [1] is utilized to perform molecular dynamics (MD) simulations.

In fig. 1 there is an example figure.

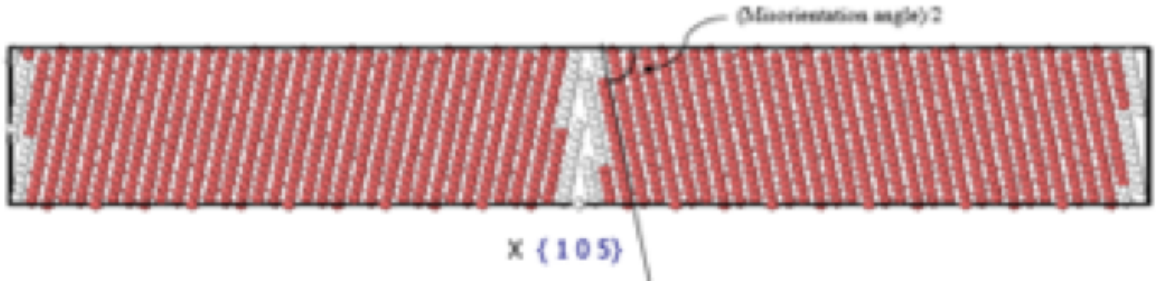

Figure 1: An example

The formation energy of point defects is calculated via equation 1:

$$E_f = E^* - \frac{n \pm 1}{n} \times E_0 \tag{1}$$

where E^* is the energy of a system with a defect (with n $\pm$1 atoms), n is the number of atoms in the defect-free system and E_0 is the energy of a defect-free system with n atoms. Equation 1 utilizes (n + 1) for interstitials and (n - 1) for vacancies.

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3. Results

3.1. Dummy title

4. Conclusions

5. Acknowledgement

This will change and we will make sure we have the right one.

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References

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