

Evaluation of the anisotropic grain boundaries and surfaces of α U via molecular dynamics

Khadija Mahbuba^a, Benjamin Beeler^{a,b}, Andrea Jokisaari^b

^aNorth Carolina State University, Raleigh, NC 27607

^bIdaho National Laboratory, Idaho Falls, ID 83415

Abstract

Abstract text

1. Introduction

Intro text

2. Computational Details

comp details text. below is Fig. 1.

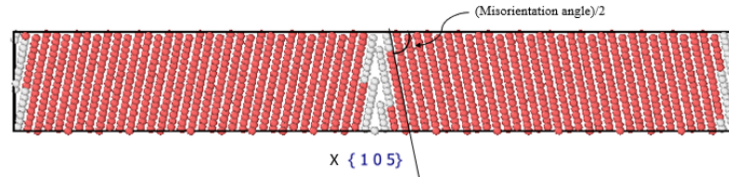


Figure 1: Caption for this Fig.

3. Results

3.1. α -U Grain Boundary Energies

3.1.1. Tilting of XY face of alpha U

3.1.2. Tilting of YZ face of alpha U

3.1.3. Tilting of XZ face of alpha U

4. Conclusions

Conclusions text

5. Acknowledgement

You can leave this for now, it will change.

Add NEAMS acknowledgement This manuscript has been authored by Battelle Energy Alliance, LLC with
15 the U.S. Department of Energy. The publisher, by accepting the article for publication, acknowledges that
the U.S. Government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce
the published form of this manuscript, or allow others to do so, for U.S. Government purposes. This research
made use of the resources of the High Performance Computing Center at Idaho National Laboratory, which
is supported by the Office of Nuclear Energy of the U.S. Department of Energy and the Nuclear Science
20 User Facilities.