# Unveiling the mechanisms of motion of synchro-Shockley dislocations in Laves phases

Zhuocheng Xie[a], Dimitri Chauraud[b,c], Achraf Atila[b,c], Erik Bitzek[b,c], Sandra Korte-Kerzel[a], Julien Guénolé[d,e]

[a]*Institute of Physical Metallurgy and Materials Physics, RWTH Aachen University, 52056 Aachen, Germany*

[b]*Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany*

[c]*Department of Materials Science and Engineering, Institute I: General Materials Properties, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany*

[d]*Université de Lorraine, CNRS, Arts et Métiers ParisTech, LEM3, 57070 Metz, France*

[e]*Labex Damas, Université de Lorraine, 57070 Metz, France*

[a]*xie@imm.rwth-aachen.de*

Synchroshear as the dominant basal slip mechanism in Laves phases is accomplished by the glide of synchro-Shockley dislocations. However, the mechanisms of motion of synchro-Shockley dislocations are still not well understood. In this work, using atomistic simulations we demonstrate that nucleation and propagation of kink pairs is the energetically favorable mechanism for the motion of synchro-Shockley dislocation. Vacancy hopping and interstitial shuffling are identified as two key mechanisms related to kink propagation. The assistance of vacancy and antisite defects on kink nucleation and propagation are investigated and shown to be crucial for kink mobility. These findings provide insights into the dependency on temperature and chemical composition of plastic deformation of topologically close-packed phases.

*Keywords: Dislocation, Laves phases, kink-pair, point defects, atomistic simulation*

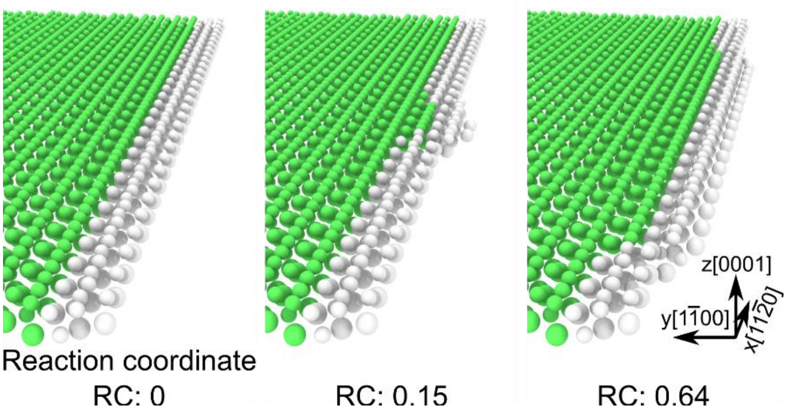


Fig.1 Transition states of kink-pair nucleation and propagation in Laves phase. Only atoms belong to stacking fault (green) and dislocation core (white) are shown here.