UNVEILING THE MECHANISMS OF MOTION OF SYNCHRO-SHOCKLEY DISLOCATIONS IN LAVES PHASES

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Key Words: Dislocation, Laves phases, kink-pair, point defects, atomistic simulation

In Laves phases, synchroshear is the dominant basal slip mechanism. It is accomplished by the glide of synchro-Shockley dislocations. However, the atomic-scale mechanisms of motion of such zonal dislocations are still not well understood. In this work, using atomistic simulations, two 30° synchro-Shockley dislocations with different Burgers vectors and core structures and energies are identified. We demonstrate that nucleation and propagation of kink pairs is the energetically favorable mechanism for the motion of the synchro-Shockley dislocation (partial I, Fig.1). Vacancy hopping and interstitial shuffling are identified as two key mechanisms related to kink propagation and we investigated how vacancies and antisite defects assist kink nucleation and propagation, which is crucial for kink mobility. Additionally, we identified a mechanism of non-sequential atomic shuffling for the motion of the synchro-Shockley dislocation (partial II). These findings provide insights into the dependency on temperature and chemical composition of plastic deformation induced by zonal dislocations in Laves phases and the many related topologically close-packed phases.

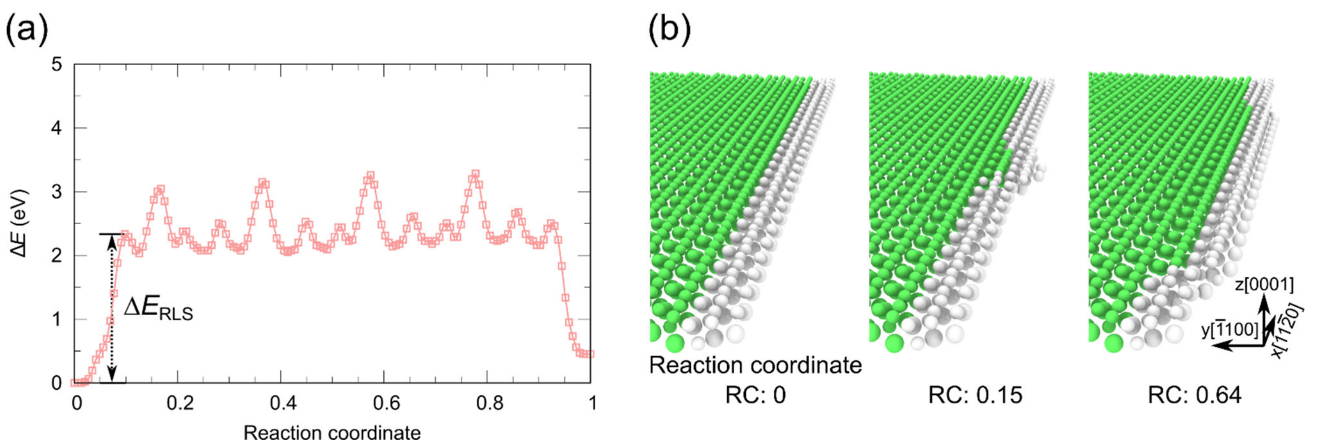

*Figure **1** – Transition mechanism of 30° synchro-Shockley dislocation motion (partial I) via kink-pair propagation in C14 $CaMg_2$ Laves phase. (a) Excess energy versus reaction coordinate (RC) is calculated using nudged elastic band. Energy profile is separated into different stages based on individual activation events. (b) Transition states of kink-pair nucleation and propagation. Only atoms belong to stacking fault (green) and dislocation core (white) are shown here.*