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Dislocations analysis of silicon crystal through action-derived molecular dynamics with tight-binding method

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Summary

We study energetics and mobility of dislocations in silicon crystal in atomistic scale. The electronic structure of silicon affects its dynamics, so that it is analyzed with tight-binding method for high accuracy, emerged as a useful method for studying structural and dynamical properties of covalent systems. The tight biding potential used for silicon crystalline is the one of GSP known as a transferable potential. Due to the nature of rare events, the analysis is executed by action-derived molecular dynamics (ADMD) calculations. The changes of the system energy due to dislocation glide are explored with a view to finding the Peierls stress and energy, which corresponds to the minimum flow stress and the activation energy barrier for dislocation movement.d then effort will be made to propose solutions to improve the results.