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MECHANICAL INSTABILITY OF CUBIC MATERIALS UNDER UNIAXIAL LOADING

Soon-Dong Park[1], Duc Tam Ho[1] and Sung Youb Kim[1]

[1] School of Mechanical and Advanced Materials Engineering, Ulsan National Institute of Science and Technology, 50 UNIST-gil, Ulsan 689-798, Korea.

*Corresponding author's email address: sykim@unist.ac.kr

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We apply the Hill's criterion to study mechanical instability behaviours of cubic crystals under uniaxial [100] loading by using density functional theory and molecular statics calculations. For this, we employ FCC metals, BCC metals, and several cubic covalent crystals such as Si, Ge and C. The Hill's criterion shows a good prediction of the instability of the FCC metals and BCC metals i.e. the symmetric bifurcation is observed at the onset of instability. However, the Hill's criterion is not valid for the prediction of the instability of covalent materials which have diamond structure, although they have the same cubic symmetry to FCC or BCC metals. Here, we discuss such abnormal behaviours of covalent materials in detail.