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DISLOCATION DIPOLES AND THE NUCLEATION OF CRACKS IN SILICON NANOPILLARS

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To understand the brittle to ductile transition at small scale in silicon nanopillars, plastic deformation of silicon nanopillars was investigated by atomistic simulations. Perfect dislocations were found to be nucleated from surfaces and nano cavities were evidenced resulting from dislocation dipoles annihilation. The formation of such cavities is consistent with previous atomistic calculations showing that the annihilation of dislocation vacancy dipole of perfect shuffle dislocations is associated to the formation of vacancy clusters in silicon and diamond [1]. In nanopillars such cavities contribute to the nucleation of cracks [2]. This mechanism of crack nucleation is relevant to single slip deformation and does not require any interactions between dislocations issued from intersecting glide planes as usually postulated for crack nucleation [3].

Incipient dipoles were also found nucleated on the glide plane swept by dislocations. These incipient dipoles result from bond flips and are similar to the Stone–Wales defects in graphene [4]. These defects could be similar and related to the “dislocations trails” found in the glide plane of dislocations in other deformation conditions, a long time and rather unsolved problem in silicon (see for example [5]). Under the applied stress those incipient dipoles appear to act as new nucleation centers for dislocations located in the glide plane. Those dislocations contribute to dislocation interactions in parallel slip planes and to the formation of nano cracks following the described above mechanism.

References

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