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Elastic instabilities in perfect crystals: from planar dislocation-like modes to diffuse buckling-like modes AKANKSHA GARG, ASAD HASAN, CRAIG MALONEY, CMU — We perform atomistic computer simulations of a model two dimensional perfect hexagonal crystal subjected to nano-indentation loading. For most crystallographic orientations, we find agreement with previous results for the case where the nearest-neighbor direction was perpendicular to the loading axis (cond-mat/1205.1700). In these orientations, the unstable mode takes the form of a sharply localized pair of atomic planes that slide relative to each other and form what is essentially a dipole of edge dislocations. The pair separation scales with the thickness of the film, L, and radius of the nanoindenter, R, in a non-trivial way that is independent of crystallographic orientation. For some crystallographic orientations with high surface energy, such as when the nearest-neighbor direction is co-incident with the loading axis, we find a new failure mode that emerges for very flat indenters and competes with the dislocation-like mode. The new diffuse failure mode is reminiscent of a buckling instability with a predominantly transverse character but exhibits both a nontrivial spatial extent and dominant wavelength that both depend on L and R.

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