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Amorphization of silicon crystals under shear stress GIANPIETRO MORAS, ANDREAS KLEMENZ, Fraunhofer Institute for Mechanics of Materials IWM, Germany, HIROSHI UETSUKA, Asahi Diamond Industrial Co., Ltd., Japan, MICHAEL MOSELER, LARS PASTEWKA, Fraunhofer Institute for Mechanics of Materials IWM, Germany — Phase transformations, and in particular amorphization, of crystalline silicon occur under contact loading, e.g. during indentation and scratching experiments. Little is known about shear-induced amorphization of Si, but molecular dynamics (MD) simulations recently unveiled that amorphization of diamond/diamond sliding interfaces is a mechanically driven process that is crucial to the anisotropic wear of diamond. Here, we report the results of MD simulations of Si crystals upon sliding load and compare them to analogous results obtained for diamond. Although crystalline Si is a brittle material with a diamond cubic structure, the properties of Si and C amorphous phases are strikingly different. Our simulations show that shear-induced phase transitions are also remarkably different in the two materials. In diamond, an amorphous region forms at the sliding interface and its thickness grows in time, with a rate that depends on normal load, surface orientation and sliding direction. Also in Si, a thin material region located at the sliding interface undergoes sudden amorphization when the shear stress exceeds the stability limit of the crystal. However, the thickness of such region does not grow in time due to competing amorphization and recrystallization processes. Further growth of the amorphous phase, at temperatures lower than the melting point, can only be achieved with normal loads that exceed the stability limit of the crystalline phase.

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