Atomistic Mechanisms of Shear-Induced LDA↔HDA Transformations and Shear Banding in Amorphous Silicon under High Pressures

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Abstract

Mechanisms of plastic deformations in amorphous solids, phase transformations (PTs) between different amorphous phases under hydrostatic loading, and PTs in crystalline materials under severe plastic deformations attract significant attention due to their great fundamental importance and applied potential. However, we are not aware of any publications on plastic shear-induced amorphous-amorphous PTs under pressure.

Here, we integrate sciences of severe plastic deformations of amorphous materials, strain-induced PTs in crystalline materials under high pressure, and sear banding, and extend them to study shear deformation under constant pressures in amorphous Si, shear-induced PTs from low-density amorphous (LDA) to high-density amorphous (HDA) Si, and mutual effects of PT and shear band formation using molecular dynamics simulations with the state-of-the-art Gaussian Approximation Potential. Shear deformation leads to the formation of a shear band, in which a dissipative structure of turbulent-like flow with swirls is revealed, followed by a reduction in the number of swirls via coalescence with further shearing. Increasing pressure results in LDA↔HDA PT with increasing atomic fraction of HDA due to pressure and shear, which in turn suppresses the shear banding, enabling the uniform deformation-PT at 9.8 GPa.

The simulations reveal that shear-induced LDA↔HDA PTs occur simultaneously until reaching steady state. Shear reduces the pressure for initiation and completion of LDA↔HDA PT by 4.3 and 5.1 GPa compared to hydrostatic loading, respectively. The atomic mechanism of PT differs fundamentally from that under hydrostatic loading. In bulk, Si deforms by atomic rearrangement in localized STZs with high nonaffine displacements, which trigger nucleation of HDA clusters within LDA and, concurrently, of LDA clusters within HDA, without their growth and coalescence. Despite the much larger shear and the expected atomic fraction of HDA in a shear band, a surprisingly sharp drop in atomic fraction of HDA within the shear band was discovered. It was found that this anomalous behavior is related to the change in deformation mechanism: swirls in a shear band promote reverse PT from HDA↔LDA more effectively than the direct PT. While a clear correlation between fields of the nonaffine squared displacement and the atomic coordination in the bulk is found, such a correlation in a shear band is lacking. There is no correlation between the atomic displacement and coordination number fields, both within and outside the shear band.

We developed a simple, mechanism-based analytical model that uses accumulated plastic strain rather than time, simultaneous direct-reverse PTs, pressure-dependent driving forces for both PTs, and different yield strengths of the phases. It possesses a steady-state solution depending on pressure. Both non-stationary and stationary solutions accurately describe the MD simulation results across all pressures, allowing us to determine all material parameters. A kinetic equation is also derived for pressure-induced LDA↔HDA PTs, and the stationary solution reproduces the MD simulation results correctly. Despite the large shear stresses, they surprisingly do not affect the PT kinetics. This happens because, according to atomic mechanisms, shear stresses simultaneously promote both direct and reverse PTs in different regions, resulting in negligible net effects.

Transformation-induced plasticity (TRIP) due to volume change during amorphous-to-amorphous PT is revealed. While for crystalline solids, temperature and/or stress hystereses require temperature and/or stress cycling to accumulate significant TRIP, LDA↔HDA PTs occur simultaneously, and each of them produces TRIP. Consequently, even for relatively low net atomic fraction of HDA, TRIP and stress relaxation can be significant due to a large number of back-and-forth events. An equation for the TRIP-induced deformation rate is proposed that accounts for the above results. Our findings provide deep atomistic and macroscopic insights into the coupled pressure-shear deformation and PT in amorphous Si, offering a crucial theoretical foundation for designing experiments and various engineering applications, including optimizing ultra-precision surface treatment by inducing ductile machining regimes and controlling failure in amorphous Si via pressure and PT.