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Nanoindentation-induced phase transformation versus shear plasticity in tetrahedral semiconductors

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Abstract – The interplay between shear-induced dislocation slip and pressure-induced phase transformation as incipient plastic responses in covalent semiconductors is considered.

Under high pressure, open-structured tetrahedral semiconductors transform to denser structural phases with six-fold or eight-fold coordination.[1] These phases typically have metallic character, and may further transform to metastable phases such as complex crystalline structures or amorphous structures on pressure release.

High-pressure phase transformations under nanoindentation was predicted by Gilman in 1992 to be a general feature of tetrahedral semiconductors.[2] This would offer a useful means of altering electronic properties in these materials at the nanoscale in a controlled fashion. However to date it has only been observed for two of the Group IV semiconductors, silicon (Si) and germanium (Ge).

During nanoindentation, both high hydrostatic stresses and high shear stresses develop under the indenter. Under initial, purely elastic loading, these stresses will increase continuously with increasing load, until one of them becomes high enough to activate an inelastic deformation mechanism: either phase transformation (hydrostatic stress) or conventional dislocation-based plasticity (shear stress). The ratio of hydrostatic to shear stress is fixed by the Hertzian equations. Hence, the preferred initial inelastic response for a given material will depend on the relative values of the yield stresses for that material (Fig. 1).

Can the preferred incipient response be predicted from basic material properties? The key factors governing a covalent material's resistance to shear plasticity are bond strength, bond length, and ionicity.[3] Bond length and ionicity also determine the pressure at which transition to a denser phase becomes thermodynamically favourable.[4] Drawing these theories together, it is possible to predict whether shear plasticity or phase transformation will be the favoured response.

Ge is a useful illustrative case, because the shear and hydrostatic responses are close in favourability and the incipient response can be pushed either way depending on the experimental conditions. We will present experimental evidence that nanoindentation-induced phase transformation can be promoted in at least two ways: by confining the Ge in thin film form to reduce the effective shear stress,[5] and by increasing the applied loading rate to increase the resistance to dislocation motion (Fig. 2).[6]

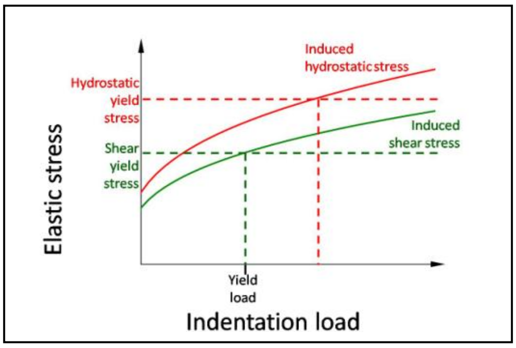

Figure 1: Plastic flow occurs when elastic stress reaches a critical yield value, corresponding to shear plasticity or phase transformation.

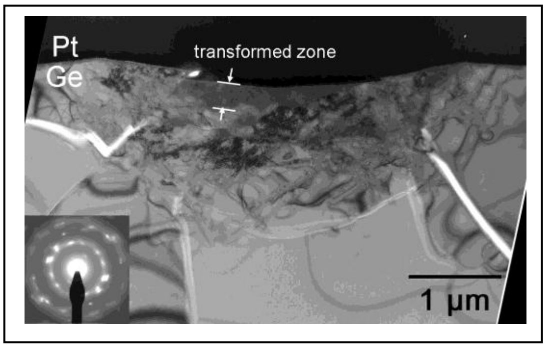

Figure 2: Transmission electron micrograph showing phase transformation in Ge after rapid loading rate nanoindentation.

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