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Fracture of single crystals having layered morphology

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Abstract. The mechanism for relaxation of elastic energy in layered crystals (where interlayer glide is possible) under a point load is discussed. Titanium dichalcogenides are chosen as materials with covalent interatomic bonds, while the Ir-Sn compound is a metallic single crystal. All studied samples have layered morphology with similar parameters, such as the thickness of the sample and the thickness of a single layer. It was found that penetration of a diamond pyramid induces mechanical twins around the indent, whereas the appearance of cracks is a very rare phenomenon. In contrast with bulk samples, cracks in layered crystals move on complicated trajectories, which do not coincide with low-index crystallographic directions. Besides, their growth is limited by the surface single layer. Gliding between neighbouring layers effectively suppresses the propagation of cracks via the interlayer boundary. Glide may be considered an irreversible shift, which prevents the fracture of a material.

1. Introduction

Irreversible (plastic) shift along the direction of tensile stress, which should hinder crack growth (Knott, 1973), occurs in materials having a macroscopic layered structure (metal-ceramics composites, multiplayer structures), but it simultaneously induces interfacial or interlayer fracture, which avoids this potential advantage of layered morphology as compared with homogeneous bulk material. On the other hand, strong adhesion between metal and non-metallic layers, which protects the sample from interfacial fracture, makes a glide of layers or the shift impossible. However, some layered crystals exhibit interlayer gliding that does not lead to interfacial fracture, but instead suppresses brittle cracks in the samples (Panfilov et al., 1998; Panfilov et al., 1999). Titanium dichalcogenides (TiX_2, X=S,Se,Te and misfit layer compounds (MLC) $(PbS)_{1.18}TiS_2$) and the Ir-Sn compound are chosen as model substances with covalent and metallic interatomic bonds, respectively, for the present work aimed at the study of stoppage of transcrystalline cracks due to interlayer shift.

2. Results

Indentation of TiS_2 crystals induced the appearance of $\langle 100 \rangle$ twin lamellas, while no cracking was revealed in the vicinity of indents in spite of severe local deformation of the material (see Figure 1a). The length of lamellas could vary, but it was always compatible with indent size (~ 0.05 mm). The depth of holes was so deep that the bottoms of the indents became invisible for a light microscope focused on the crystal surface. No other kinds of deformation tracks, such as slip bands or twins having different orientations, were observed in deformed samples. However, long straight cracks whose lengths are of the order of the sample size and whose growth directions never coincide with any low-index crystallographic direction sometimes appeared near the places where bending stresses have maximal value. Their growth never led to a failure of the layered crystal, inasmuch as they advanced in the surface layer only.

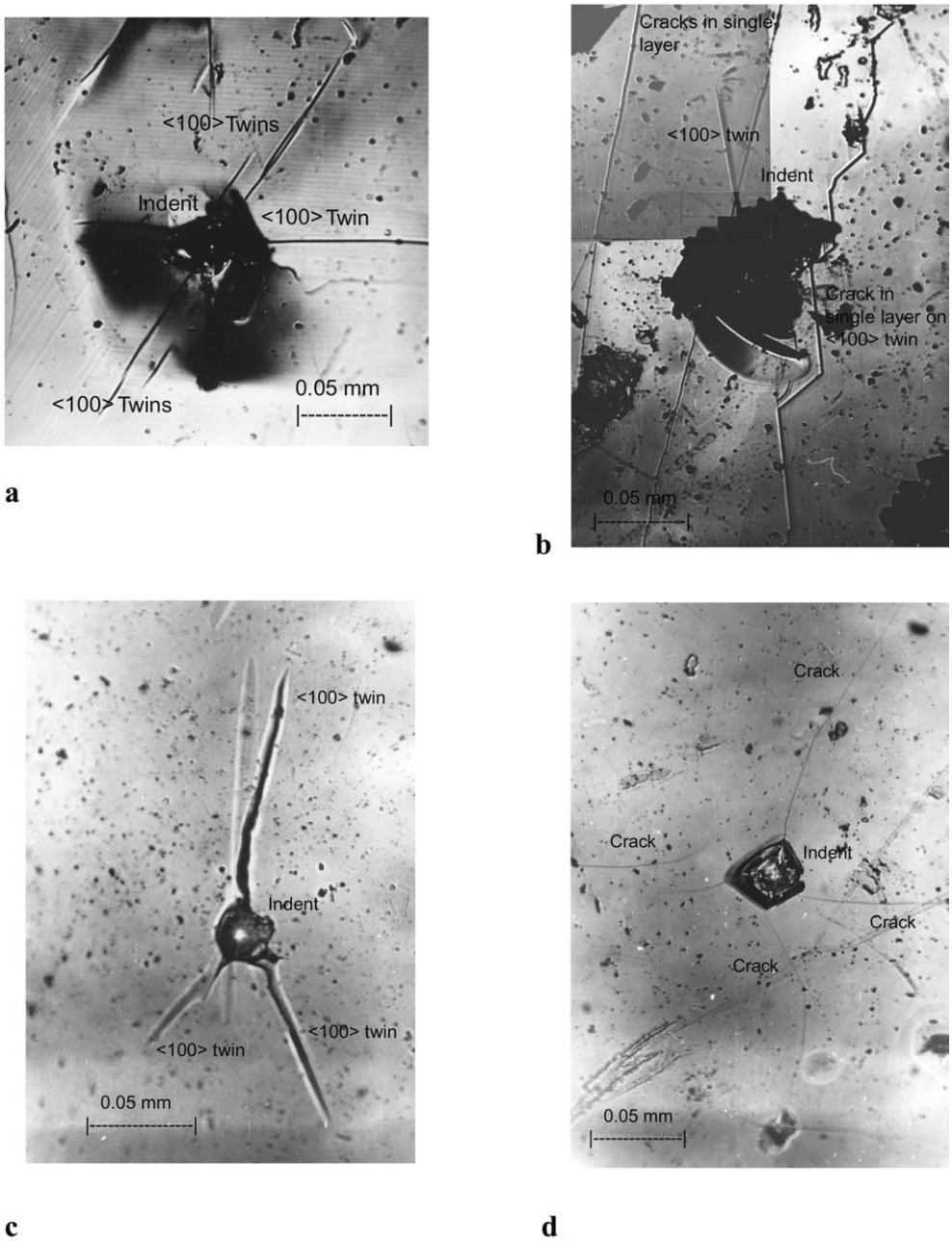

Figure 1. Indentation of TiX_2 crystals: a – TiS_2, b – $TiSe_2$, c – twins in $TiTe_2$, d – cracks in $TiTe_2$.

As a rule, point load did not induce mechanical twinning and cracks in $TiSe_2$ crystals, although sometimes twins were observed near large indents (Figure 1b). In comparison with TiS_2, lamellas were two to three times longer, but their quantity was much less. Bending of $TiSe_2$ crystals also led to the appearance of long cracks, which advanced within the surface single layer and never caused separation of the sample. These cracks possessed either straight or broken profiles; however, their motion coincided with a low index ($\langle 100 \rangle$) direction when the crack was moving along twin lamella. Indentation of $TiTe_2$ mainly induced mechanical

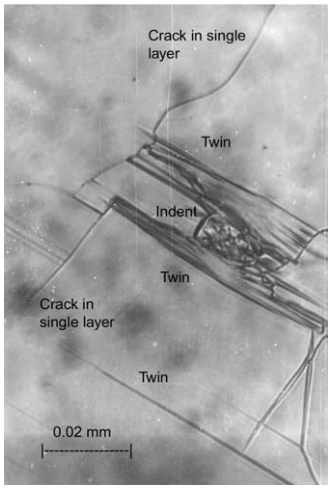

Figure 2. Indentation of $(PbS)_{1.18}TiS_2$.

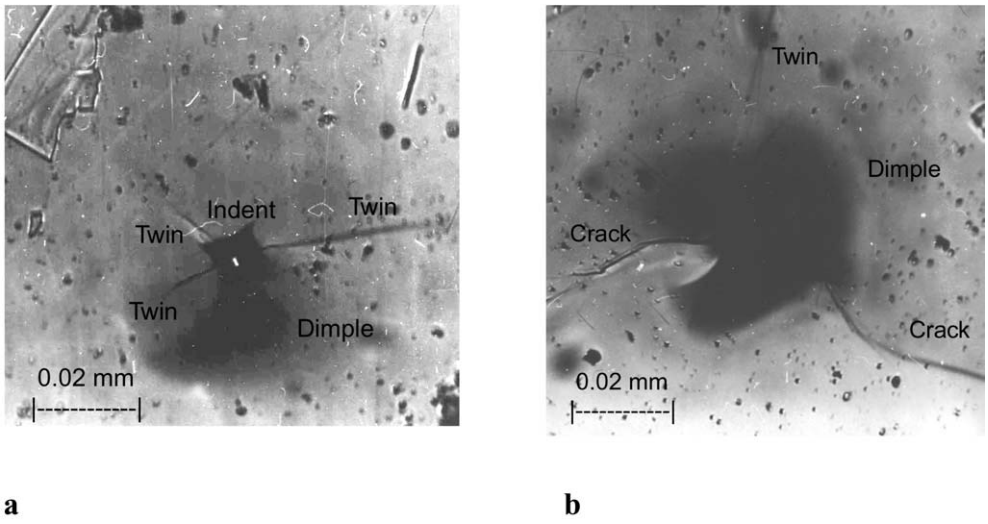

Figure 3. Indentation of Ir-Sn compound: **a** – twins near indent in Ir-Sn crystal; **b** – cracks near indent.

twins along ⟨100⟩ direction, whose length was two to three times longer than the diagonal of the indent (Figure 1c). The next visible channel for accommodation of elastic energy was cracks that moved on complicated trajectories in the surface single layer (Figure 1d). In contrast with other titanium dichalcogenides, both indentation and bending of $TiTe_2$ crystal could lead to separation of the parts of the surface layer. Perhaps this feature may be connected with the fact that $TiTe_2$ has the weakest interatomic cohesive strength among titanium dichalcogenides.

Due to the complicated structure of Lauegrams, the twin direction in MLC $(PbS)_{1.18}TiS_2$ was not determined; however, metallographic observations have shown that all twin lamellas oriented along the sole direction. No long cracks with straight profile were detected on MLCs. The rolling of samples by finger caused the appearance of deformation twins and thin curvilinear lines on their surfaces, and the quantities of twin lamellas and lines (and their width) increased with their deformation degree rising. According to estimations, the depth of the lines

was of the order of a single layer thickness (10^{-4} mm). These objects may be considered as cracks in the single layer that appeared due to interlayer glide (Panfilov et al., 1998). Two sets of twins induced by the point loads surround every indent, while cracks were not observed in this place (see Figure 2). Sometimes the curvilinear lines came close to these twins, but it does not mean that indentation created them.

Penetration of the diamond pyramid into the Ir-Sn samples led to the appearance of a deep dimple around indents (Figure 3). No twin lamellas, slip bands and other deformation defects were revealed on the surface surrounding the dimples, since all cracks and ⟨110⟩ twin lamellas induced by point load were localized in the limit of the dimple area. Cracks moved on complicated trajectories, which could coincide with low index (⟨100⟩ and ⟨110⟩) directions on the initial stage of evolution only. At that their growth was limited by the surface layer, as in previous cases.

3. Discussion

As was shown, all tested layered crystals exhibit similar behaviour. Mechanical twinning is the main visible channel for accommodation of elastic energy under a point load, whereas cracking occupies only the second position. This is a normal kind of response for metallic-type material; however, such behaviour is not inherent for bulk crystals having directed (covalent) interatomic bonds, where indentation always induces cracks. Trajectories of cracks in layered crystals also differ from ones in bulk crystals, whose cracks have a tendency to advance along low-index crystallographic directions. However, the basic difference between our layered samples and bulk crystals is the limitation of transcrystalline crack growth in the surface single layer. Cracks could not pass through the interlayer boundary even when the point load begins to cause interlayer failure of the sample.

Hence, there should be some mechanism for suppression of crack growth on the interlayer boundary. Dislocation motion, which is an effective engine for such a process, is forbidden in titanium dichalcogenides because of covalent bonds and in Ir-Sn because of a small c/a ratio. Therefore, the irreversible shift of the neighbouring single layers under applied stress remains the sole mechanism able to suppress crack growth. Such a shift is visible in MLC, where it has almost ‘macroscopical’ magnitude. According to measurements of crack width under rolling, it may be varied in the limits of 10^{-3} mm. In so doing, the shifting of layers did not lead to interlayer failure of the sample. In other crystals, long cracks do not change their width under rolling and bending; but it does not mean that irreversible shift is absent, since cracks are also arrested on interlayer boundaries here. In other words, the shift or gliding of layers without interlayer fracture is the third channel, which absorbs the main part of elastic energy and suppresses transcrystalline crack growth under indentation. The main features of the behaviour of tested layered crystals do not depend on the type of interatomic bonds. This is the expected result, since all samples possess similar morphology and mechanical properties (for example, the deformation process inside single layers does not connect with the motion of perfect dislocations, and mechanical twinning is the main deformation mechanism inside a single layer).

Acknowledgement

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