Dislocation microstructure in strontium titanate plastically deformed at low temperature

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$SrTiO_3$ is one of the most important perovskite oxides, since it is widely used by semiconductor technology. The mechanical behavior of $SrTiO_3$ single crystals was studied over a wide range of temperature (46-1811 K) and a ductile-to-brittle-to-ductile transition (DBDT) was found [1, 2]. This work is focused on the range below room temperature. Weak-beam dark-field (WB-DF) TEM observations of $SrTiO_3$ deformed with the compression axis along <100> below room temperature reveal a dislocation microstructure composed principally of long straight ***a***<011> screw dislocation segments (Fig. 1), in agreement with previous observations [2–4]. Furthermore, most screw dislocations are arranged in narrow dipoles. By trace analyses using large-angle tilt the dipole habit plane was found to be close to (100), which is in agreement with what elasticity theory predicts for screw dislocations. However, the dipole width is between 5 and 15 nm, implicating an interaction stress of the order of several GPa which is clearly in excess of the critical resolved shear stress on the {100} plane. Therefore annihilation of the screw dislocations should be expected. The restricted mobility exhibited at these temperatures by these screw segments suggests that some process is operating on the dislocation core structure reducing drastically its mobility.

In order to reveal such processes high resolution TEM was used to investigate the core of ***a***<110> screw dislocations. Figure 2 shows a very frequently observed structure. No inserted atom planes are visible, but two narrow segments parallel to the {110} plane are observed (limited by the arrows in Fig. 2). This arrangement is consistent with a dislocation dipole where both screw dislocations are dissociated into two partial screw dislocations with ***b***=***a***/2<110>, bordering a stacking fault on the {110} plane. From the dissociation width (3 ± 0.2 nm) a stacking-fault energy of 480 ± 30 mJ/m^2 is deduced. The two dissociated dislocations are separated almost parallel to the (100) plane by about 6 nm which is in very good agreement with the WB-DF results shown above. Also the separation of the partial dislocations is close to what Zhang et al. [5] found for dissociated edge **a**<110> dislocations. This makes sense because the stacking fault plane is the same. Moreover, the dissociation plane is also {110}, which is the plane of minimal stacking fault energy [6].

Due to the core structure shown in Fig.2 the partials cannot easily glide out of their slip planes. This is particularly so because of the large stacking fault on non-{110} planes. Hence, the annihilation process for this dipolar configuration is extremely impeded even under the high stresses coming from the interaction forces between dislocations, and therefore very narrow screw dipoles can be observed.

It is worth emphasizing that due to the small dissociation width up to now ***a***<110> dissociated dislocations have not been observed by WB-DF in strained specimens of $SrTiO_3$. Figure 2 is a clear proof that a dissociation process of ***a***<110> screw dislocations takes place, which allows formation of very narrow dipoles. Although the reason for the restricted mobility of long screw segments is not explained yet, in some way the dissociation process discussed above must be involved.

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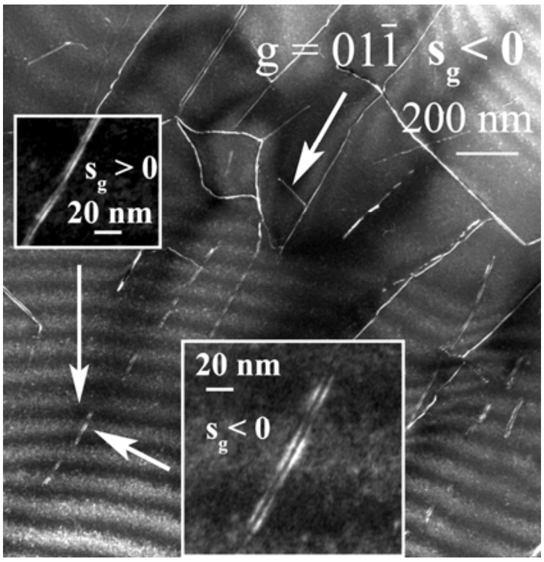

Figure 1. Micrograph of $SrTiO_3$ strained ~ 3% at 113 K along the <100> compression axis, showing long straight screw segments and very narrow dipoles. The foil is parallel to the {011} plane, but here it is tilted ~ 50° around the $[01\bar{1}]$ direction.

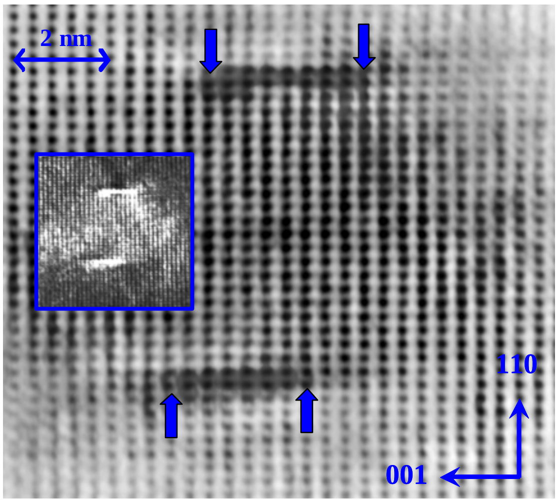

Figure 2. High-resolution TEM micrograph of $SrTiO_3$ deformed at 149 K along the <100> compression axis. The view is along the <110> direction and a dipolar configuration comprised by two ***a***<110> screw dislocations is observed. Each one is dissociated into two ***a***/2<110> partials.

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