892 CD
DOI: 10.1017/S1431927606062489
Microsc Microanal 12(Supp 2), 2006

Dislocations in strontium titanate

W. Sigle*, D. Brunner*, Z. Zhang**, S. Taeri***, C. Sarbu****

*Max Planck Institute for Metals Research, Heisenbergstraße 3, D-70569 Stuttgart, Germany
**Fritz Haber Institute, Dept. of Inorganic Chemistry, Faradayweg 4-6, D-14195 Berlin, Germany
***Amselweg 11 , D-71706 Markgröningen, Germany
****National Institute for Materials Physics, Magurele–Bucharest, Romania

Strontium titanate is an oxide ceramic with perovskite structure. Despite the seemingly simple cubic crystal structure the plastic behaviour (under compression) recently turned out to exhibit quite a spectacular ductile-to-brittle-to-ductile transition shown in Fig.1 [1,2]. Above 1500 K (Regime C) the flow stress is strongly temperature dependent with an activation energy of about 6 eV. The temperature dependence is much less pronounced below 1000 K (Regime A) where the flow stress is low and slightly increases towards low temperatures. In between (Regime B) the material fails by brittle fracture at stresses increasing with increasing temperatures without yielding.

By conventional and weak-beam TEM we found the following dislocation structures [3,4]: *Regime A*: Dislocations have Burgers vector *a*<110>, irrespective of the deformation axis. Whereas edge dislocations are predominant at the high-temperature end, straight screw dislocations dominate towards the low-temperatures end (113 K). *Regime B*: Dislocations are constrained within small isolated bundles, separated by dislocation-free regions. *Regime C*: Dislocations have *a*<110> Burgers vectors, predominantly of edge-type, if the material is compressed along the 'hard' <100> direction, and *a*<100> Burgers vectors if compression is performed along directions different from <100>.

To summarize, there are at least four puzzling findings:

1) Why is the flow stress much lower in Regime A than in Regime C although the same slip system is active?
2) Why does the material fracture and why does this happen at a well-defined, but temperature-dependent stress?
3) Why does the flow stress increase in Regime A towards low temperatures?
4) Why are dislocations with *a*<100> Burgers vector not present in Regimes A and B for non-<100> compression axes?

We believe that most of these puzzles can be resolved by a model based on the structure of dislocation cores. A key feature is that at elevated temperatures *a*<110> edge dislocations tend to dissociate by a climb mechanism into two partial dislocations with Burgers vector *a*/2<110>. This is supported by high-resolution TEM results obtained from bi-crystals [5]. The dissociation by climb is easily possible only in Regime C. However, such a dissociation prevents the dislocation from gliding. Instead, it has to climb requiring high activation energies. Within Regime B the climb dissociation is not accomplished over the whole dislocation length. Furthermore, thermal activation is not sufficient to induce climb of the dissociated segments, rendering them sessile. In regime A, temperature is too low for climb dissociation. Therefore no sessile segments are present and the dislocation can move by normal glide at relatively low stress levels. The flow stress increase towards low temperatures is probably related to the core structure of screw dislocations because these show very straight appearance, much like in bcc metals.

Irrespective of the Burgers vector, we did not succeed in observing dislocation dissociation by the weak-beam technique. This is surprising considering the large magnitude of the <110> Burgers vectors. As noted above we found dissociation of a<110> dislocations in low-angle grain boundaries by high-resolution TEM [5]. The partial separation was 2.5 nm which is close to the resolution limit of the weak-beam technique. These results show that the {110} antiphase boundary energy is high and a value of (720 ± 280) mJ/m^2 was deduced from the HRTEM data.

Apart from the plastic behaviour, dislocations in $SrTiO_3$ also have strong influence on the charge transport properties. Electron energy-loss spectra acquired from the dislocation cores confirm that the dislocation cores are non-stoichiometric, showing a higher Ti-to-O ratio as compared to the bulk material [5, 6]. That this non-stoichiometry leads to a charged dislocation core was confirmed by impedance spectroscopy studies performed on a bi-crystal containing a low-angle grain boundary [7]. These data show a blocking effect of the low-angle grain boundary against oxygen ion diffusion. This is explained by a positively charged dislocation core which is surrounded by a space-charge zone. Variation of the separation of the dislocations leads to different barrier heights of the low-angle grain boundaries [8].

[1] D. Brunner et al., J. Am. Cer. Soc. 84 (2001) 1161.
[2] P. Gumbsch et al., Phys. Rev. Lett. 87 (2001) 085505-1.
[3] S. Taeri et al., Z. Metallkd. 95 (2004) 433.
[4] W. Sigle et al., submitted to Phil. Mag. (2006)
[5] Z. Zhang et al., Phys. Rev. B66 (2002) 214112.
[6] Z. Zhang et al., Phys. Rev. B66 (2002) 094108.
[7] R. A. de Souza et al., J. Am. Ceram. Soc. 86, No.6 (2003) 922.
[8] R. A. de Souza et al., J. Appl. Phys. 97 (2005) 053502.
[9] The financial support by the German Science Foundation is gratefully acknowledged (GRK285).

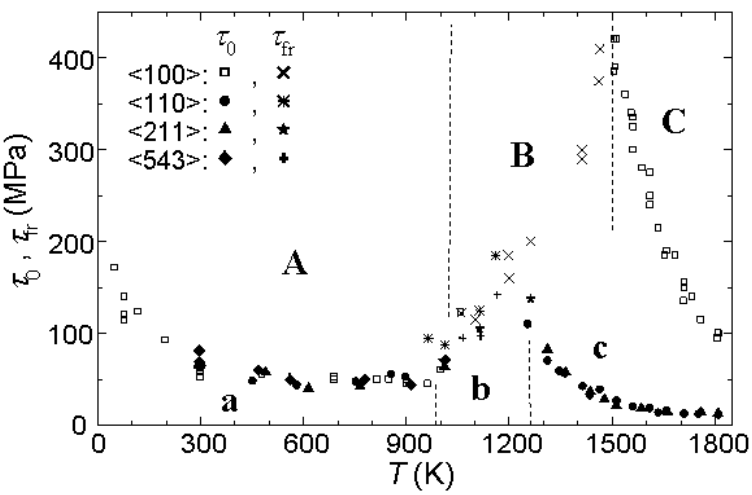

Fig.1: Temperature dependence of the flow stress, τ_o, and fracture stress, τ_{fr},of $SrTiO_3$ under compressive loading along different crystallographic axes. The classification labels (A, B, C) shown in the upper part of the Figure are for the <100> compression axis, whereas those shown in the lower part (a, b, c) are for orientations other than <100>. The low-temperature flow stresses coincide for all orientations, but the temperature range of Regime B and the high-temperature flow stresses in Regime C are orientation-dependent. This is related with the different glide systems: The easy glide system a<100>{100} which is active for non-<100> compression in Regime C cannot operate with a load parallel to <100> because of the vanishing Schmid factor.