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The predicted 3-D atomistic structure of an interfacial screw–edge dislocation

Dean C. Sayle

Department of Environmental and Ordnance Systems, Cranfield University, Royal Military College of Science, Shrivenham, Swindon, UK SN6 8LA. E-mail: sayle@rmcs.cranfield.ac.uk

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Atomistic computer simulation techniques have been employed to generate an amorphous SrO thin film on an MgO(100) substrate, which, under dynamics simulation, recrystallises revealing misfit induced structural modifications including mixed screw–edge dislocations, lattice slip and twist boundaries.

The presence of an interface between two dissimilar materials can induce defects, which govern the chemical and physical properties of the material. Clearly, the structural characterisation, formation mechanism, and exploitation of such defects to generate optimised material properties are highly desirable and remain central to industries, ranging from catalysis and semiconductor to civil engineering. Here we show how defects including twist boundaries; slip; edge and screw dislocations within a supported metal oxide can be explored using simulation techniques. Experimental techniques for studying 'interfacial' defects have enabled almost atomic resolution and in conjunction with simulation, detailed models have been proposed.[1] Conversely, the defect structures identified here were not artificially constructed based on experimental images; rather the structures *recrystallised*, from an amorphous structure. Consequently, fully characterised three-dimensional atomic structures of such defects were generated and are presented, using molecular graphics. Surprisingly, the dislocations demonstrate almost 'textbook' structural simplicity.

In a previous study,[2] ultra-thin films of CaO on SrO were grown by sequentially depositing Ca and O species onto an SrO(100) substrate. Inspection of the resulting interfaces revealed significant structural features within the thin film, which help accommodate the lattice misfit associated with the system. Moreover, by increasing the size of the simulation cell, additional structural features, which were too large to be accommodated within the smaller simulation cell, were observed. Certain structural features, such as supported grain-boundaries, can be very large, necessitating the use of a suitably large simulation cell. Accordingly, in this present study we increase the size of the simulation cell. However, the deposition method, used previously, is very computationally expensive. Consequently, in this study an alternative method for generating the thin film interface, which reduces considerably the computational expense, is presented.

The MARVIN code[3] was used to perform all the atomistic simulations presented in this study including energy minimisation and dynamics simulation. The code considers the crystal as a stack of ions periodic in two dimensions. The stack is subdivided into two regions: a region I, where all the ions are allowed to relax explicitly, and a region II, where the ions are all held fixed relative to each other. Region II is included to ensure that the long-range effects of the ions in the bulk of the crystal on the surface region are correctly represented. The top of region I is the free surface, onto which ions, comprising the thin film, are positioned to generate the interface. To reduce the computational cost, region I for the support was two layers thick.

The interionic potentials employed were based on the Born model of the ionic solid in which the ions interact *via* long-range Coulombic interactions and short-range, parameterised interactions and were taken from Lewis and Catlow.[4] In addition, a rigid ion model was used to reduce the computational expense.

The SrO/MgO(100) interface was constructed by placing four SrO(100) layers directly above an MgO(100) support with the SrO constrained to occupy 'on top' positions thereby accommodating the entire +20% misfit associated with this system. The size of the simulation cell was 28 × 28 which corresponds to 28 atoms or 14 MgO repeat units for each side of the supercell. Each MgO layer therefore comprises 784 atoms, which is over five times larger than the '12 × 12' cell used previously. Dynamics simulation was then applied to the system followed by energy minimisation at 0 K.

The structure of the SrO/MgO thin film was inspected at various intervals during the dynamics simulation. After 5 ps at 2100 K, the structure of the SrO thin film was completely amorphous, while after 25 ps certain SrO regions started to recrystallise into the rocksalt structure [Fig. 1(a), (b)]. The average Sr–O bond distances (after 25 ps), monitored by calculating the radial distribution function (RDF) for the Sr–O within the amorphous film was *ca.* 2.5–2.6 Å, which compares with 2.57 Å for pure Sr–O (and 2.1 Å Sr–O distances of the starting configuration). This suggests that there was much less strain within the amorphous SrO thin film compared with the starting configuration. The thickness of the SrO thin film also increased from 8.4 Å for the initial configuration to *ca.* 20–22 Å for the amorphous film.

During prolonged dynamics simulation, further recrystallisation of the SrO occurred until the whole of the thin film could be characterised as crystalline. The dynamics simulation was run for a total of 150 ps at 2100 K followed by 90 ps at 1500 K in an attempt to generate a low energy configuration and finally energy minimised at 0 K. The dynamics simulation required *ca.* 11 days on a Silicon Graphics Origin 2000 using 26 R12,000 processors.

For many simulations the starting configuration is likely to influence the final structure. Moreover, there is a danger, particularly within incommensurate interface systems, of generating structures which may be artefacts of the initial configuration. Conversely, in this study, the SrO thin film recrystallised from an amorphous phase in which the SrO accommodated its natural lattice parameter, eliminating any possible influence or '*memory*' of the starting configuration.

We now consider the structural features of the resulting thin film interface.

Inspection of the final structure of the SrO/MgO interface (Fig. 2) reveals that the SrO thin film comprises *ca.* six to seven layers (17–20 Å thick) with an average interplanar distance of *ca.* 2.6 Å. The Sr–O distances (RDF) were calculated to range from 2.4 to 2.8 Å with an average of *ca.* 2.6 Å, which compares with 2.57 Å for the natural Sr–O bond distance. The surface

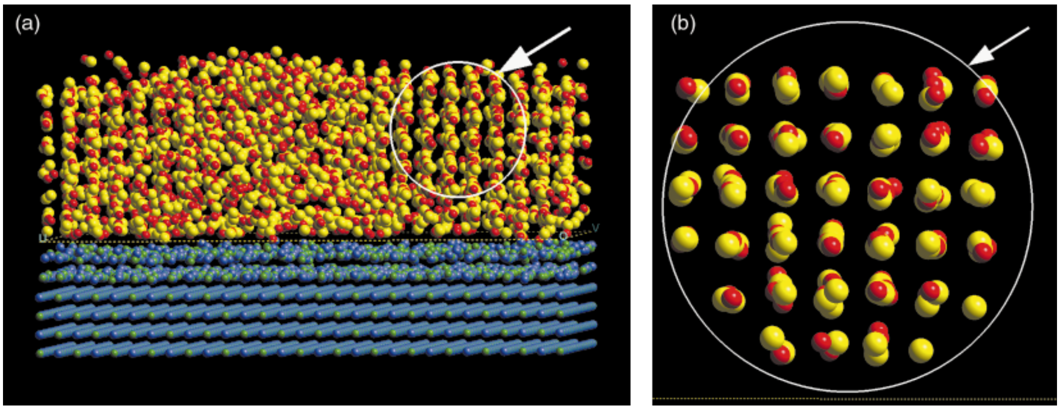

Fig. 1 (a) Representation of the SrO/MgO(100) simulation cell after 25 ps of dynamics simulation. The circle on the figure highlights a region of the SrO, which has started to recrystallise into the rocksalt structure; (b) an enlarged spherical region of the SrO thin film depicting the 'recrystallised' SrO. To aid interpretation, the SrO is projected at a slightly different angle, compared with (a), to emphasize more clearly the rocksalt structure. Strontium is coloured yellow, magnesium is blue, oxygen (SrO) is red and oxygen (MgO) is green.

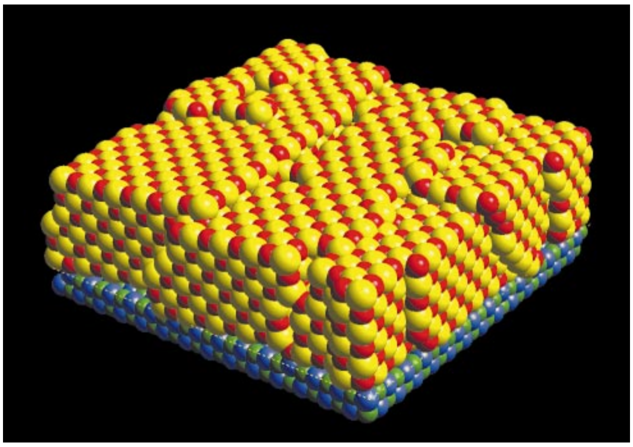

Fig. 2 Representation of the final structure of the SrO(100)/MgO(100) interface. Only two planes of the MgO support have been included for reasons of clarity. Colour notation as in Fig. 1.

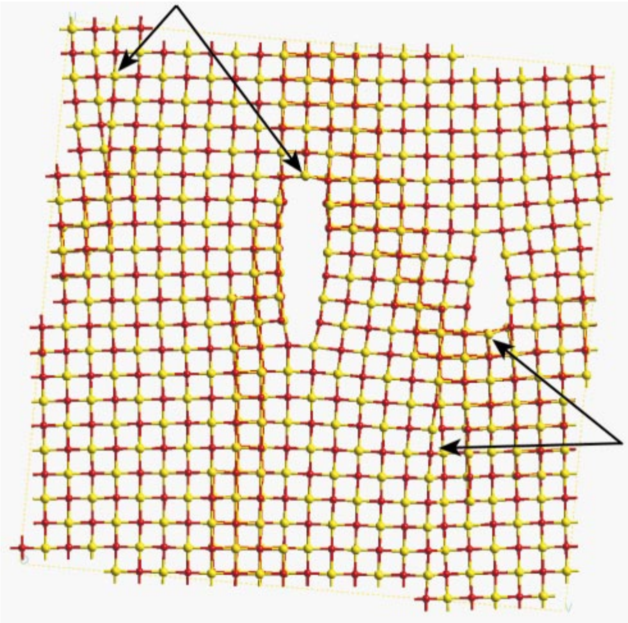

Fig. 3 Ball and stick representation of a slice, cut parallel to the interface, through the SrO thin film. Colour notation as in Fig. 1. The arrows indicate the location of the four dislocations.

energy of the interface was calculated to be 2.4 J m^{-2}, which is comparable to interface energies calculated previously.[2]

The SrO thin film exposes steps at the surface, which indicate the presence of dislocation arrays.[5] In particular, Fig. 3 depicts a slice, parallel to the interfacial plane, through the SrO, which reveals four dislocations within the SrO thin film. Inspection of the 'void' at the centre of Fig. 3 revealed a dislocation (Fig. 4), which traverses almost the entire thickness of the SrO thin film. To aid interpretation, two additional representations have been depicted [Fig. 5(a), (b)]. Directly to the right of this dislocation (Fig. 3) an additional dislocation was observed [Fig. 6(a), (b)].

Burgers vectors, which can easily be assigned to each dislocation by inspection of the structures in Fig. 5(a) and 6(a), lie at *ca.* 45° to the line of the dislocation. This indicates that the dislocations have both screw and edge character.

Fig. 7 depicts, more clearly, the edge component of the dislocation and reveals also that the SrO is rotated with respect to the MgO support about an axis perpendicular to the plane of the interface. Fig. 8 depicts a slice cut perpendicular to the interface and demonstrates slip of the SrO lattice planes and Fig. 9 presents the structure of the 'screw–edge' dislocation after 100 ps superimposed on the final structure (240 ps).

In summary, this study demonstrates how models of interface structures can be generated using atomistic computer simulation techniques. In particular, the thin film was recrystallised from an amorphous structure, which enables

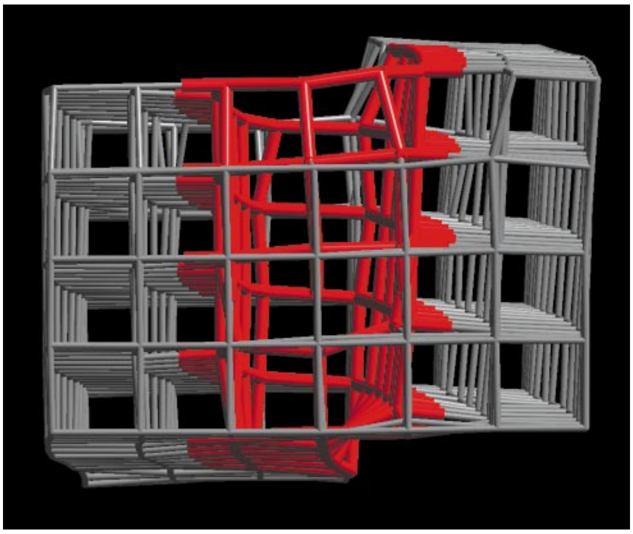

Fig. 4 Stick representation of the screw dislocation within the SrO thin film. The red sticks depict the spiral of atoms within the dislocation helix, while the grey sticks represent part of the surrounding SrO lattice.

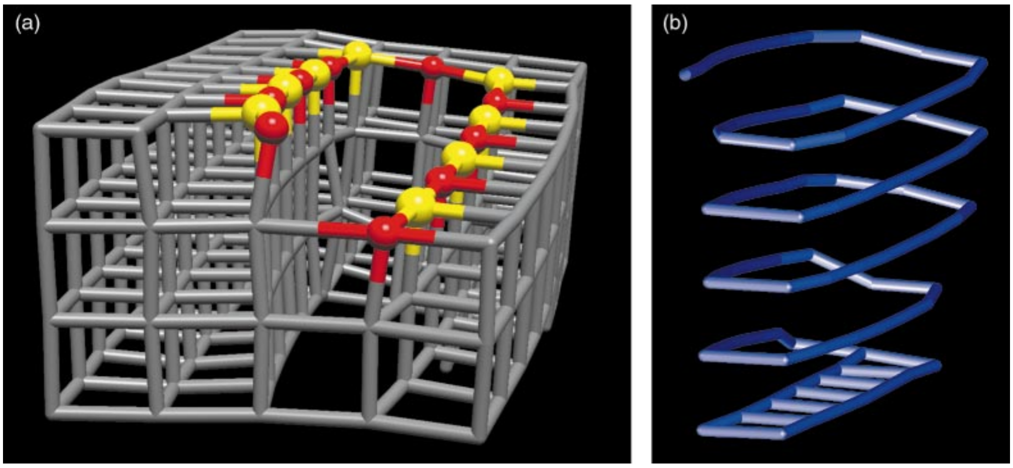

Fig. 5 Representations of the screw dislocation depicted by the void located at the centre of Fig. 3; (a) representation of part of the SrO lattice (coloured grey) which surrounds the screw dislocation; (b) stick representation of the spiral of atoms. Colour notation as in Fig. 1.

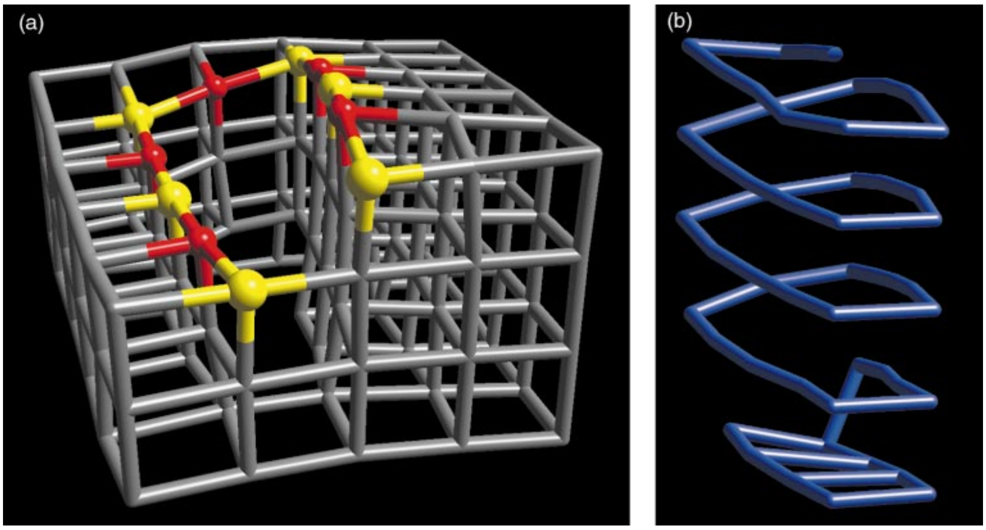

Fig. 6 Representation of the screw dislocation depicted by the void to the right of centre in Fig. 3. Notation as in Fig. 5.

the system to lose any 'memory' of the starting configuration. Consequently, this approach eliminates the possibility of the structural modifications observed being an artefact of the starting configuration. The procedure was considerably faster than previous studies, where the interface was constructed *via* the sequential deposition of atoms,[2] allowing a much larger simulation cell to be employed (albeit at a cost of losing information on nucleation and growth mechanisms). Consequently, structural modifications including twist boundaries, lattice slip and screw–edge dislocations were observed. Moreover, the core structures of the screw–edge dislocations were observed to be up to 20 Å long; previous simulation cells were insufficiently large to accommodate such structures and were therefore not observed. The driving force for the evolution of such structural modifications is attributed to reducing the lattice misfit between the two materials.

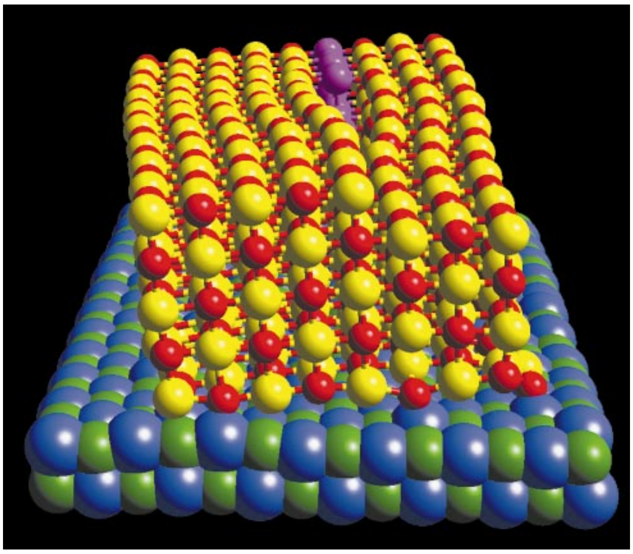

Fig. 7 Representation of part of the SrO crystal supported on the MgO depicting, more clearly, the edge component of the screw–edge dislocation (atoms in purple). Colour notation as in Fig. 1.

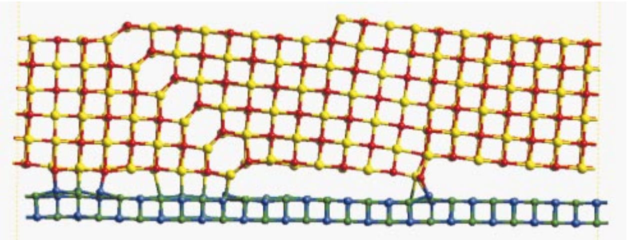

Fig. 8 Ball and stick representation of a slice, cut perpendicular to the interface, depicting slip within the SrO lattice. Colour notation as in Fig. 1.

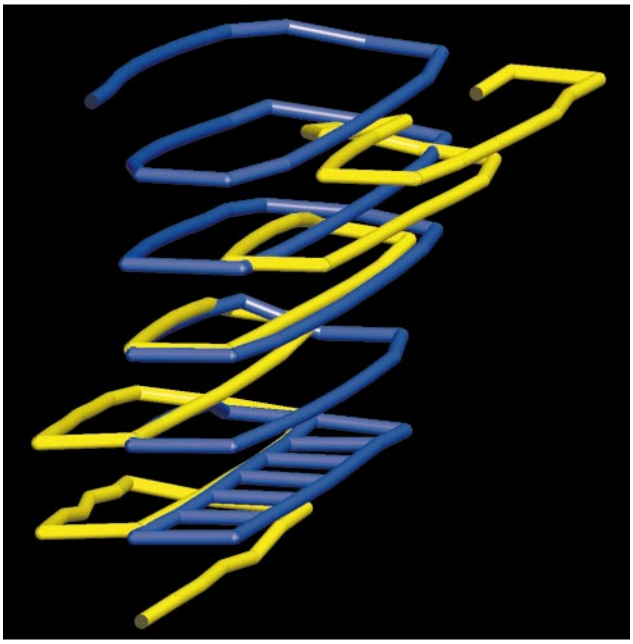

Fig. 9 Stick representation of the screw–edge dislocation after 100 ps (yellow) superimposed on the final structure (blue) of the dislocation.

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