Atomistic Structure of the Equilibrated Ni(111)-YSZ(111) Solid-Solid Interface

Technion – Israel Institute of Technology
Department of Materials Science & Engineering

Russell Berrie Nanotechnology Institute
המכון לננוטכנולוגיה ע"ש ראסל ברי

Hadar (Bratt) Nahor and Wayne D. Kaplan
Department of Materials Science and Engineering, Technion , Haifa, Israel

Introduction

The stability of metal films on oxide surfaces is important for the performance of devices such as solid oxide fuel cells (SOFCs) and thermal barrier coatings (TBCs) [1-3]. Ni-YSZ serves as an anode material in SOFCs, where the three-phase boundaries (Ni/YSZ/fuel-gas) are essential for catalytic activity which controls the electrical properties.

Numerous studies have been performed in the past regarding the coherency state of different metal-ceramic interfaces having a wide range of lattice mismatches, where many studies have focused on the fcc metal-MgO interface as a model system . Different interfaces with lattice mismatch up to ~17% were found to be semi-coherent [4-7].

In this study, fully equilibrated Ni-YSZ(111) interfaces were produced by dewetting in a reducing atmosphere and investigated using aberration corrected microscopy. The detailed analysis provided interesting findings regarding the coherency state at the interface; despite the large lattice mismatch, the interface was found to be semi-coherent and contained a misfit dislocation array. Hence, it can be deduced that the coherency state is determined not only by the lattice mismatch, but also by the lateral symmetry at the interface [8].

Experimental Methods

Dewetting Experiments

YSZ substrates (99.99%) with a surface parallel to (111) were provided by MaTeck Material Technology & Crystal GmbH. The polished substrates were ultrasonically cleaned in acetone and ethanol. A ~150 nm thick Ni film was deposited on the substrates by e-beam evaporation. After deposition, solid-state dewetting was conducted at 1350˚C (0.94 T_m of Ni) in Ar+H_2 99.9999%, at $P(O_2)$ =10^{-20} atm for 6 hr [9].

Characterization

A dual beam focused ion beam (FIB) equipped with a nano-manipulator was used for preparation of TEM specimens from the center of particles with a known morphology and orientation using the "lift out" technique [10, 11].
A monochromated and aberration (image) corrected high resolution TEM (HRTEM; FEI Titan 80-300) was used to study the orientation relationship between the Ni particles and the YSZ substrate and to acquire phase contrast micrographs of the interface region. Simulated images were generated by multislice simulations (using the software EMS [12]) and quantitatively compared to the experimental micrographs using the cross-correlation coefficient [13] .

Results and Discussion

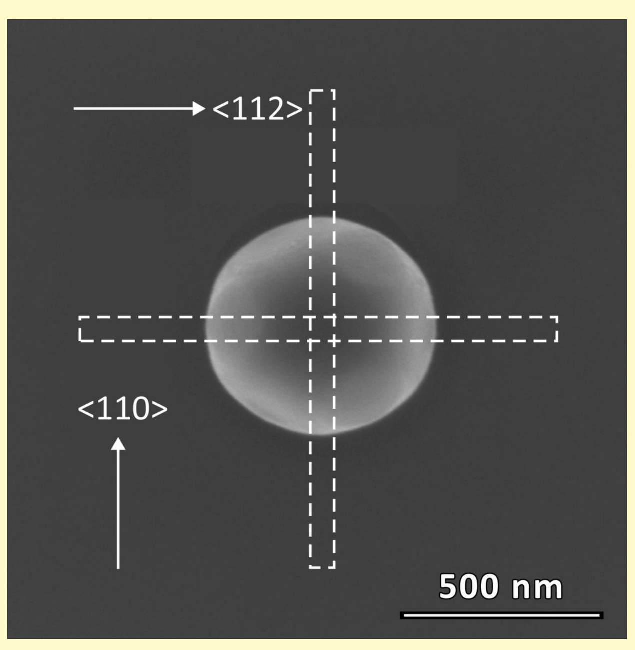

Figure 1: HRSEM micrograph of an equilibrated single-crystal Ni particle on the (111) substrate, oriented with the (111) plane parallel to the substrate surface. The dashed rectangles indicate the locations and directions of FIB sectioning.

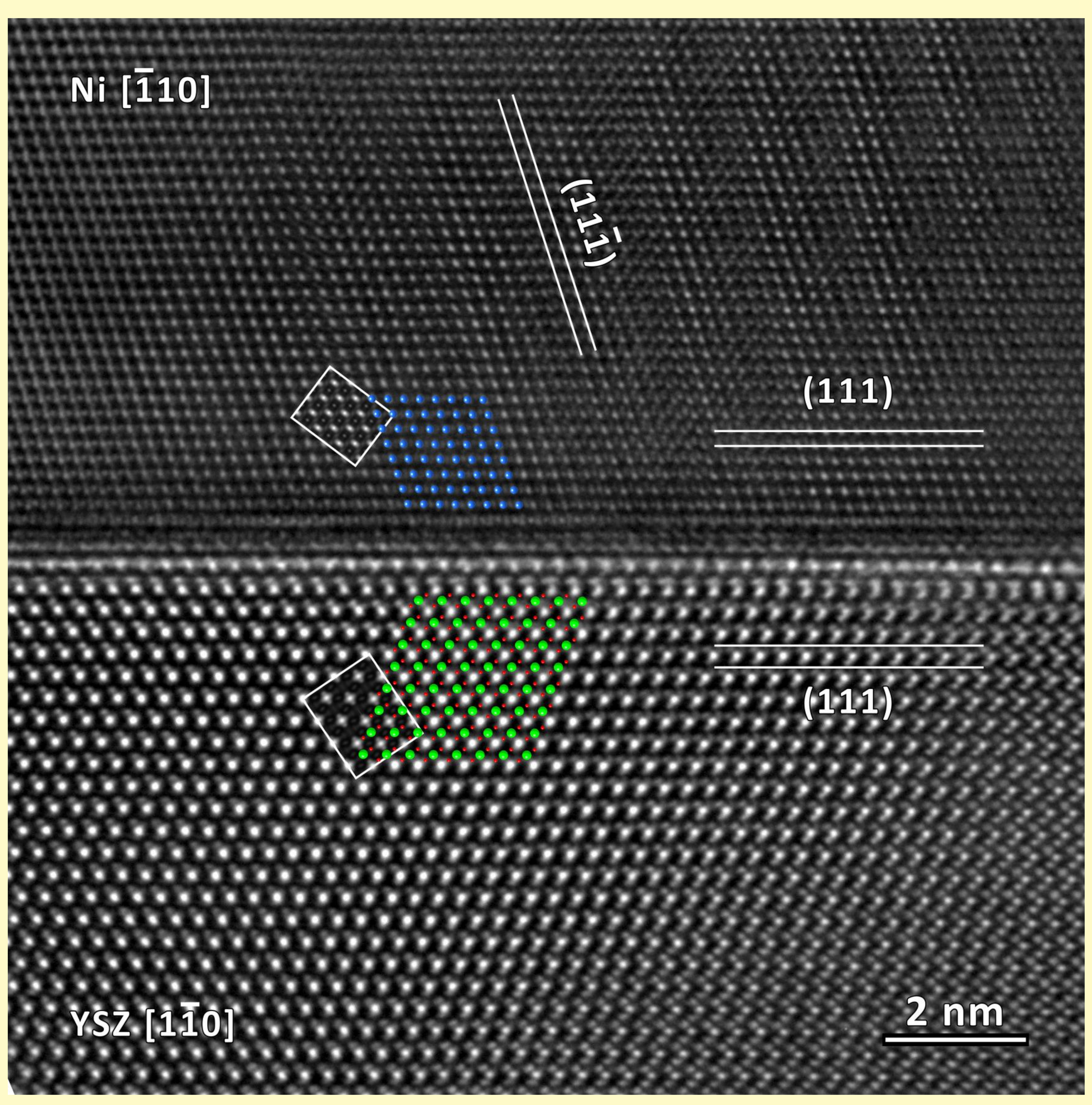

Figure 2: HRTEM micrograph acquired from the interface region of an equilibrated Ni particle along the [110] projection (sectioned according to Fig. 1, in the direction labeled as <110>). The simulated Ni and YSZ images are inset and the resulting atomic positions are overlaid for both bulk phases (Ni: blue, Zr: green, O: red). Bending of the   planes is observed next to the intersection of these planes with the interface.

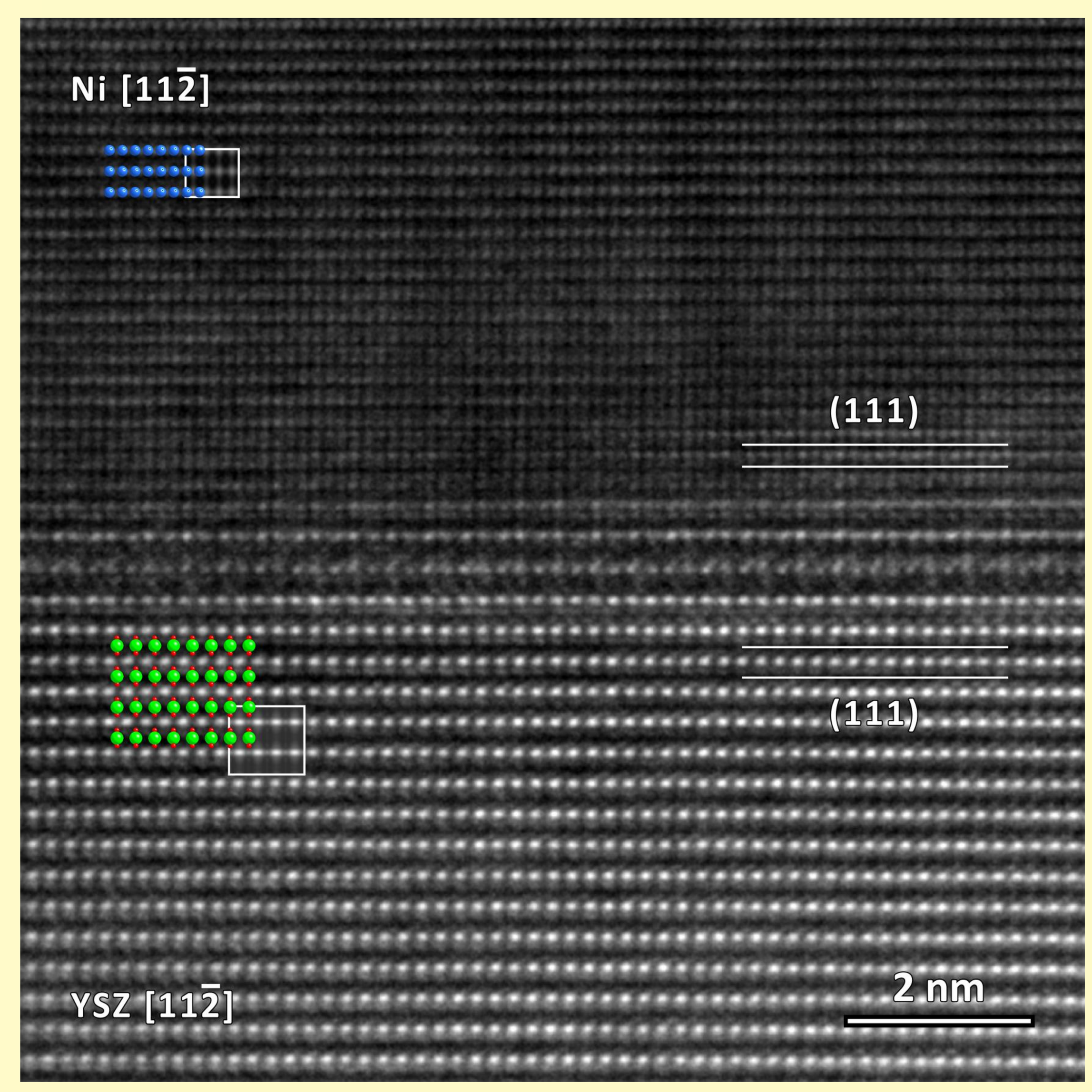

Figure 3: HRTEM micrograph acquired from the interface region of an equilibrated Ni particle along the [112] projection (sectioned according to Fig. 1, in the direction labeled as <112>). The simulated Ni and YSZ images are inset and the resulting atomic positions are overlaid for both bulk phases (Ni: blue, Zr: green, O: red).

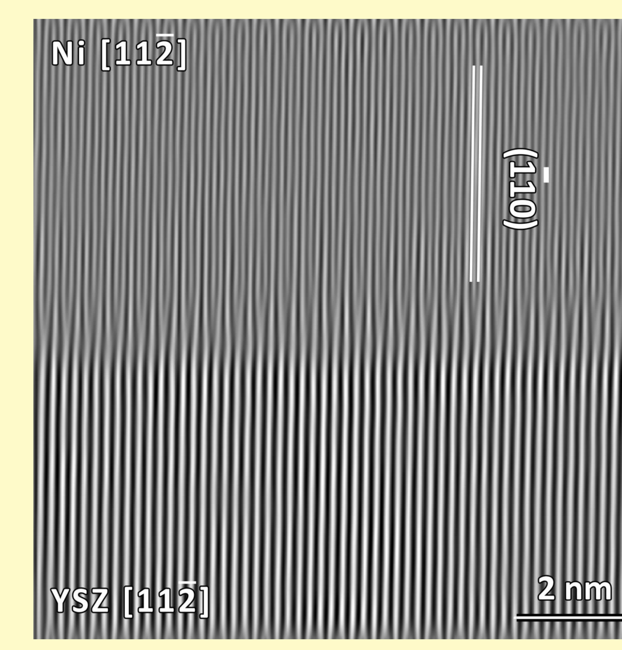

Figure 4: Bragg filtering of Figure 3 using the [110] diffraction points both for Ni and YSZ. Bending of the Ni [110] planes adjacent to each dislocation is clearly seen next to the intersection of these planes with the interface.

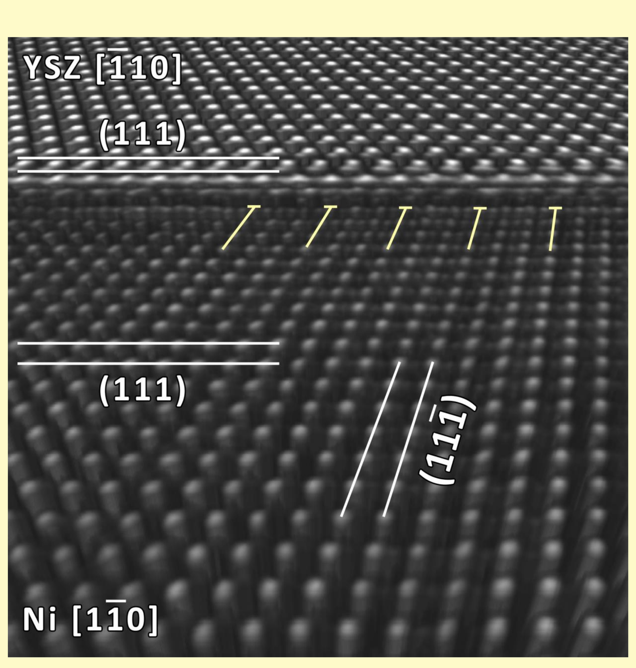

Figure 5: HRTEM micrograph acquired from the interface region of an equilibrated Ni particle along the Ni [110] projection. To enable observation of the Ni edge (misfit) dislocations at the interface, the micrograph is inclined. Some edge dislocations are marked.

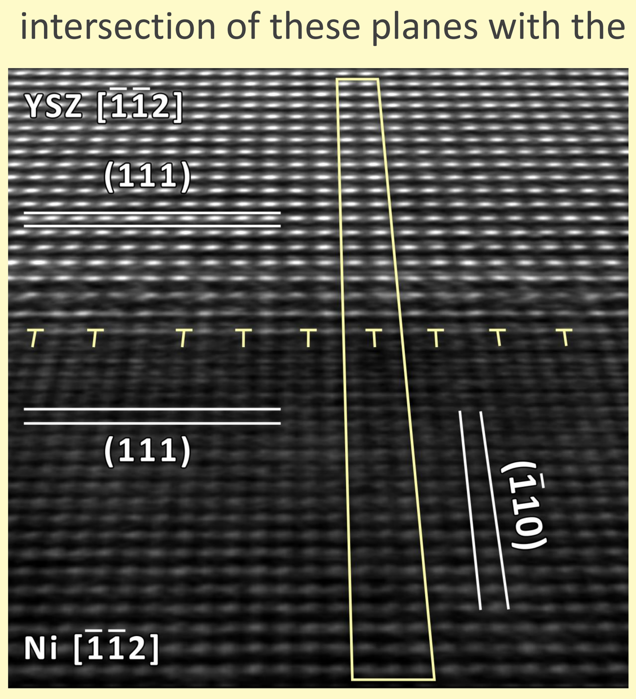

Figure 6: HRTEM micrograph acquired from the interface region of an equilibrated Ni particle along the [112] projection. To enable observation of the Ni edge (misfit) dislocations at the interface, the micrograph is inclined. One edge dislocation is framed.

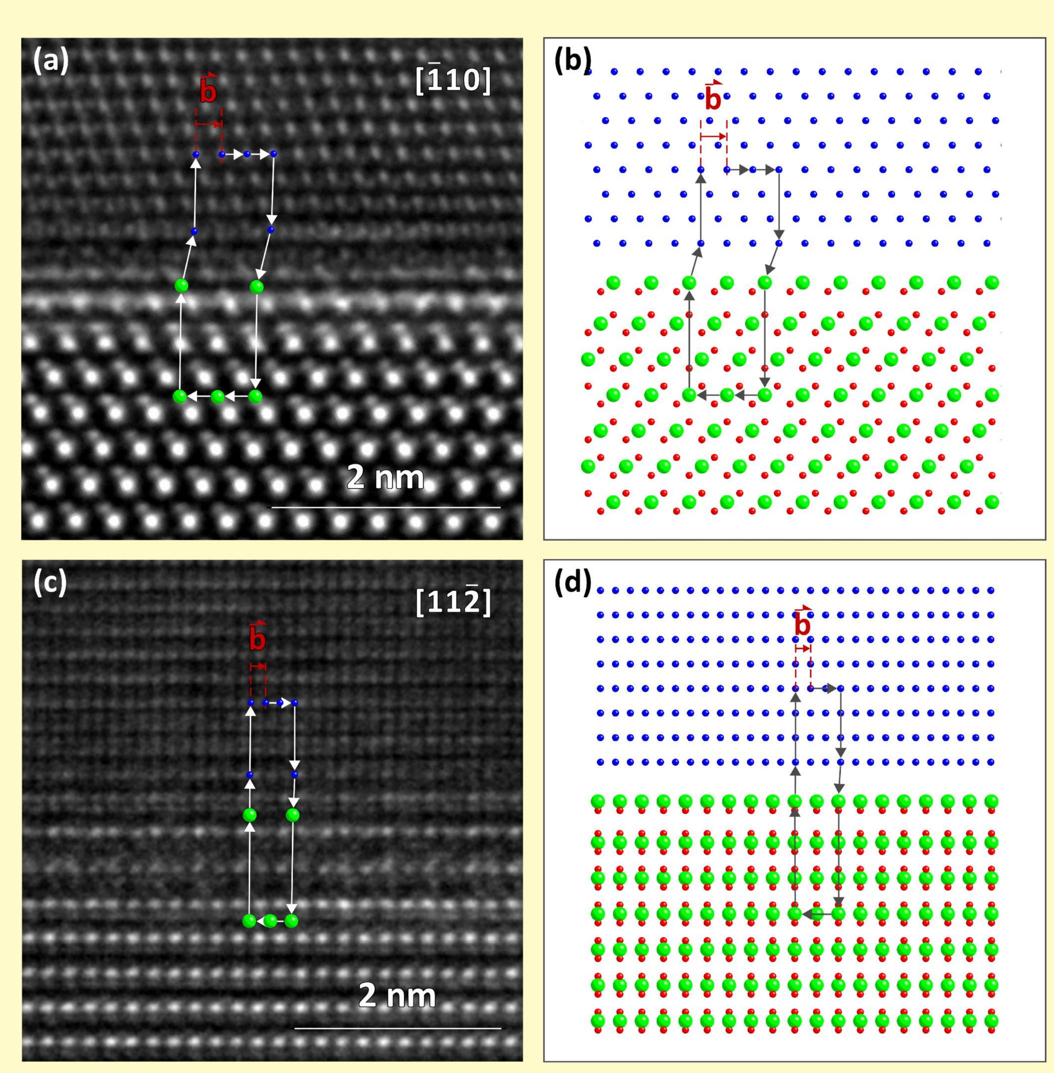

Figure 7: (a,c) Magnified images of the interface region presented in Figures 2 (a, b) respectively. Closed clock-wise circuits have been drawn around the misfit dislocations. Burgers vectors of the misfit dislocations at the interface are indicated. The Burgers vector observed in the [110] zone axis is [112], and the Burgers vector observed in the [112] zone axis is [110]. (b,d) The same Burgers vectors are indicated on the corresponding models.

Summary and Conclusions

Aberration corrected HRTEM was used to analyze the structure of the fully equilibrated Ni[110](111)‖YSZ[110](111) interface. Despite the large lattice mismatch (31%) between Ni and YSZ, the interface was found to be semi-coherent and a 2D network of misfit dislocations was identified. Based on experimental evidence supported by atomistic simulations, it can be concluded that the coherency state is determined not only by the lattice mismatch, but also by the lateral symmetry at the interface [9].

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