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The Electronic Structure of Grain
Boundaries in Nb

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ABSTRACT

We present first-principles calculations of the electronic structure of Nb grain boundaries. These are the first such calculations for a bcc metal using the real-space multiple-scattering theory (RSMST). Local densities of states near a $\Sigma 5$ twist grain boundary are compared to those for bulk Nb.

INTRODUCTION

The real-space multiple-scattering theory (RSMST) has been used [1, 2] to perform electronic-structure calculations at $\Sigma 5$ grain boundaries in fcc Cu. In this paper, we present the results of RSMST electronic-structure calculations at the $\Sigma 5$ (100) 36.9° twist grain boundary in bcc Nb. This represents a significant extension of the method, because the bcc structure is more open than the fcc structure, and in Nb the Fermi level lies inside the *d*-bands.

Since the RSMST has been described in previous publications[1, 3, 4], we shall forgo all but a very brief description of this method here. The RSMST is based on the concept of semi-infinite periodicity (SIP), defined as the regular repetition along a given direction of a scattering unit (atom, planes of atoms, etc.), or a set of such units. Systems with SIP possess the property of removal invariance, which states that the scattering properties (scattering matrices) of any such system remain invariant when an integral number of scattering units is removed from, or added to, the free end of the system. Using this property in conjunction with multiple-scattering theory, one can determine the electronic Green function, and hence all one-particle quantities such as the density of states (DOS), directly in real space, bypassing often cumbersome reciprocal-space (*k*-space) integrations, and avoiding artificial periodic boundary conditions. This formalism provides a unified treatment of the electronic properties of a broad spectrum of systems that includes, but is not limited to, pure elemental solids, compounds, ordered alloys, surfaces and interfaces, and other low-symmetry systems. Only systems with no recognizable periodic structure, e.g. amorphous materials and liquids, fall outside the scope of the RSMST method.

The essence of the method consists in a prescription for the proper renormalization of the scattering properties of the boundary sites of a cluster of atoms. Unrenormalized or "bare" sites in the interior of the cluster describe the region of interest, such as a grain boundary, while the renormalized boundary sites represent the infinite medium surrounding the cluster. This "dressing up" of the cluster is done independently for each part of a system that is characterized by its own SIP, so that grain boundaries between essentially arbitrary crystal structures can be treated. At its present stage of development, our codes can be applied to known atomistic configurations with known electronic one-particle potentials. Work currently in progress is aimed at the incorporation of the often important effects of charge self-consistency, and of total-energy capability, into the program.

In the calculations reported here, we used the self-consistent potentials for bulk Nb given by Moruzzi, Janak and Williams (MJW) [5]. The atomic coordinates of the unrelaxed grain boundaries are easily found through an appropriate twisting or tilting of one half of the underlying lattice.

Figure 1 displays the local electronic DOS's corresponding to a coincidence site (a site which is common to the lattices on both sides of an interface) at both an unrelaxed and a relaxed $\Sigma 5$ (100) 36.9° twist grain boundary in Nb. The bulk Nb DOS, calculated with the RSMST, is also displayed for comparison. (This bulk DOS reproduces the main features of the MJW calculation; small differences may be attributed to our use of a coarser energy grid and a small imaginary component of the energy.) The unrelaxed grain-boundary DOS exhibits smearing of structure compared to the bulk DOS, because of the loss of periodicity and the associated destruction of the Van Hove singularities. The grain boundary DOS is broader than that of the bulk material due to the decreased distance between some of the Nb atoms across the interface. (In fact, simply twisting one half of the crystal with respect to the other results in some of the atoms overlapping across the boundary).

Fig. 1. — Electronic density of states associated with a coincidence site at a $\Sigma 5$ (100) 36.9° twist grain boundary in Nb. DOS's for the unrelaxed and relaxed configurations are shown, respectively, as solid curves in panels (a) and (b), and are compared with those of bulk Nb (dotted curves).

Both the atomistic and electronic characteristics change noticeably in the case of the relaxed grain boundary. We expect the dominant effect of relaxation to be an expansion at the boundary layer. As in the case of Cu₂[2] we have taken a 20% expansion. The structure of the relaxed grain-boundary DOS is sharper than the DOS at the unrelaxed grain boundary.

As the calculations just presented illustrate, the RSMST method allows one to obtain the electronic structure of materials with extended defects, such as surfaces and interfaces, on an atom-by-atom basis. It has been demonstrated to work on both fcc and bcc metals, even in the case of partially-filled *d*-bands. Although in its present stage our code is slower than those based on conventional methods when applied to systems of high symmetry, it holds the distinct advantage of being applicable to low-symmetry structures that are not amenable to treatment by these methods. We are currently attempting to increase the efficiency of our code and add charge self-consistency and total-energy capabilities.

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