

18th Intern Conf. of Physics of Semicond  
P. 351 World Ser. 351  
1987

Electronic Structure and Interface States of the  
(100)Fe/Ge Interface

W.E. Pickett and D.A. Papaconstantopoulos

Naval Research Laboratory  
Washington, DC 20375-5000  
USA

ABSTRACT

We present calculations of the electronic states of the (110)Fe/Ge interface using tight-binding parameters derived by fitting to spin-polarized Fe bands, pseudopotential Ge bands and CsCl-structure FeGe bands. We utilize a generalized Slater-Koster scheme suitable for complicated geometries and capable of handling a large number of atoms per unit cell with realistic computational effort. Our results show that the Fe minority spin projected band structure has interface bands that lie in the fundamental gap of Ge; and that the majority spin has a large number of interface states just above the Fermi level strongly localized on the Ge atoms. These results are consistent with the reactive nature of this Fe/Ge interface shown by experiments.

1. INTRODUCTION

Metal-semiconductor interfaces are of considerable technological interest and therefore have stimulated several experimental and theoretical studies. In this work we report calculations of the electronic structure of the (110)Fe/Ge interface. These calculations were motivated by the work of Prinz et al.<sup>1-3</sup> who, using molecular beam epitaxy, have grown single crystal (110)Fe films on GaAs but found that Fe films grown on Ge are heavily intermixed with Ge to a thickness of several tens of layers. In our study we determine the electronic states of the non-relaxed (110)Fe/Ge interface using a supercell geometry. We

find minority interface bands which lie in the Ge energy gap, and a large density of majority spin interface resonances near the Fermi level  $E_F$ .

## 2. METHOD OF CALCULATION

The (110) interface requires 4 Fe and 2 Ge atoms per respective layer. In order to isolate the interface bands it was necessary to use 7 layers of Fe and 11 layers of Ge for a total of 50 atoms. Present day computer capabilities make such a calculation practically impossible from first principles. For this reason our calculations were done with the parametrized tight-binding method of Slater and Koster,<sup>4</sup> using a general computer code<sup>5</sup> that allows an arbitrary unit cell which can be periodically repeated in zero, one, two, or three dimensions. The tight-binding parameters needed in this approach were found by fitting to the energy bands of the host elements Fe and Ge, with a three neighbor orthogonal basis in the two-center approximation.<sup>6</sup> In addition we determined the Fe-Ge interaction parameters by fitting to the energy bands of a hypothetical CsCl-structure FeGe compound. Adjustment of the energy scale of this calculation was made via the on-site tight-binding parameters, to place  $E_F$  in the middle of the Ge gap (as suggested by experiments<sup>7</sup> on Ge-metal systems) and to eliminate unphysical charge transfer between atoms near the interface.

## 3. RESULTS AND DISCUSSIONS

In Fig. 1 the minority spin local densities of states (LDOS) are shown for several planes. The shaded lines indicate areas where the LDOS exceeds the bulk DOS. This excess LDOS appears mainly near  $E_F$  with very little elsewhere.

The majority spin LDOS is shown in Fig. 2. As is indicated by the shaded areas large excess LDOS is found on Ge in its fundamental gap. These states are metal-induced gap states like those observed at many other metal-insulator interfaces.

The excess LDOS can be understood qualitatively if we consider that an Fe atom at the interface has only half of its first two bcc

shells occupied by Fe atoms. It is only when the Fe atoms are surrounded by all first- and second-neighbors that the bonding-antibonding separation characteristic of the bcc structure occurs. In the same way in Ge the energy gap forms only if several neighboring shells are all occupied by Ge. Thus independently of the specific geometrical arrangement of atoms, a large LDOS at the interface should occur near the gap/Fermi level.

Our results for the ideal geometry show a rich spectrum of minority interface states in the mutual gap, and large majority LDOS on the Ge atoms at the interface. The large interface DOS at  $E_F$  suggests that the system may gain electronic energy by intermixing<sup>3</sup> to form a disordered interface or an interfacial compound. This notion seems to be consistent with the experimental evidence for intermixing at the interface when Fe is deposited on the Ge surface.<sup>3</sup> A more detailed account of this work will be given elsewhere.<sup>8</sup>

This work was supported by Office of Naval Research Contract No. N0014-83-WR-30007.

#### 4. REFERENCES

1. Prinz, G.A. and Krebs, J.J., Appl. Phys. Lett. 39, 397 (1981).
2. Hathaway, K.B. and Prinz, G.A., Phys. Rev. Lett. 47, 1761 (1981).
3. Prinz, G.A. and Krebs, J.J., unpublished.
4. Slater, J.C. and Koster, G.F., Phys. Rev. 94, 1498 (1954).
5. Pickett, W.E., unpublished.
6. Papaconstantopoulos, D.A., "Handbook of the Band Structure of Elemental Solids", Plenum, New York 1986.
7. Sze, S.M., Physics of Semiconductor Devices (J. Wiley & Sons, New York, 1981).
8. Pickett, W.E. and Papaconstantopoulos, D.A., Phys. Rev. to be published.

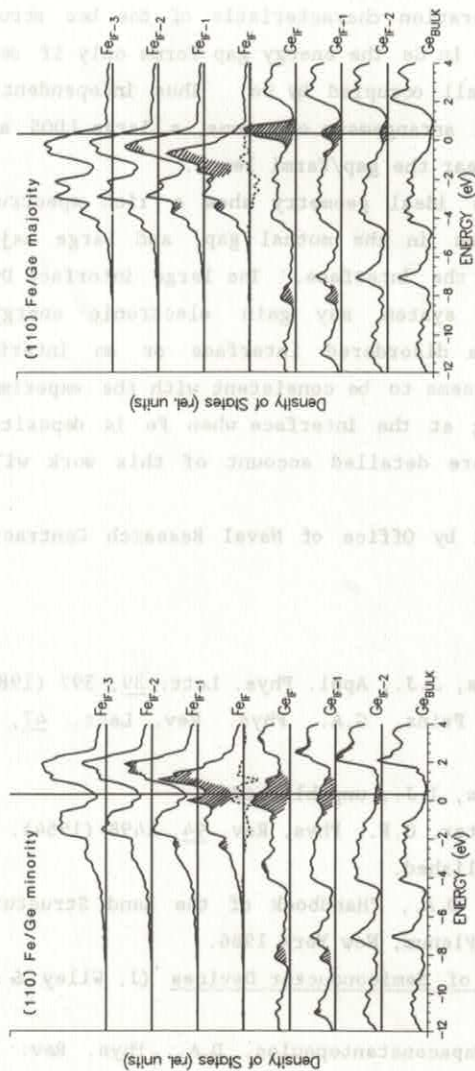


Figure 1. The minority local density of states (LDOS) per atom on several Fe and Ge layers near the Fe/Ge (110) interface. The hashed region indicates interface states, i.e. where the LDOS exceeds the bulk DOS. "GeBULK" indicates an average over the interior five layers of Ge. The dotted line on the Fe<sub>F</sub> layer indicates the difference between the LDOS on the Fe<sub>F</sub><sup>↑</sup> and Fe<sub>F</sub><sup>↓</sup> sites. Note: the LDOS for the Ge layers have been multiplied by two for easier comparison.

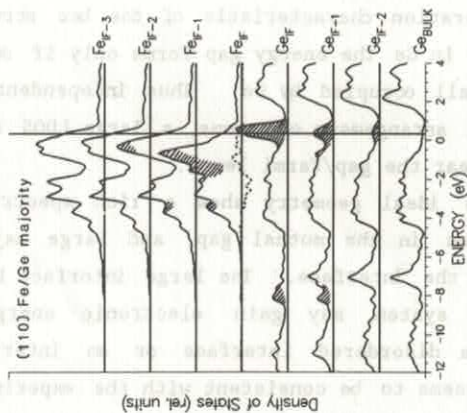


Figure 2. As in Figure 1, but for the majority spin.