Title
NEW SURFACE STATES OF AN UNRELAXED (110) SURFACE

Authors
Joannopoulos, J.D.
Cohen, Marvin L.

Publication Date
1974-08-01

Submitted to Physics Letters

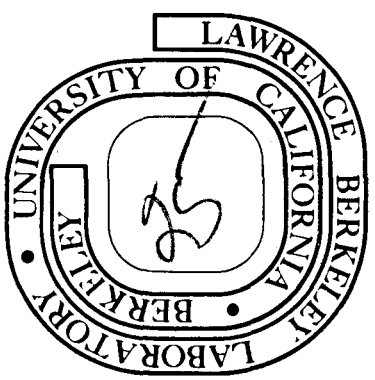
LBL-3129
Preprint c.2

NEW SURFACE STATES OF AN UNRELAXED (110) SURFACE

J. D. Joannopoulos and Marvin L. Cohen

August, 1974

Prepared for the U. S. Atomic Energy Commission
under Contract W-7405-ENG-48



LBL-3129
c.2

DISCLAIMER

New Surface States of an Unrelaxed (110) Surface*

J. D. Joannopoulos† and Marvin L. Cohen
Department of Physics, University of California and
Inorganic Materials Research Division, Lawrence Berkeley Laboratory
Berkeley, California 94720

Abstract

Electronic densities of states are calculated using a simple tight binding model for an unrelaxed (110) surface of Ge and GaAs. New surface states for Ge and GaAs are found near the bottom of the valence bands.

We have calculated local[1] and total electronic densities of states for unrelaxed (110) surfaces of Ge and GaAs using simple tight binding models. These are the first calculations on a (110) surface using a method similar to that used by Hirabayashi and others on (111) surfaces.[2-4] It involves using an sp^3-like tight binding Hamiltonian and including all interactions between nearest neighbor atoms in a system consisting of a finite number N layers of atoms in one dimension and a periodic infinite number of atoms in the other two dimensions. Very reliable results can be obtained with only $N \geq 10$. In our calculations we have taken $N = 12$ with 5 interaction parameters for Ge and 6 for GaAs. The details of our calculations and parameters used will be discussed elsewhere.[1]

In Figs. 1(a) and 1(b) we show the total density of states of the Ge and GaAs system respectively. These are unsmoothed computer plots and the small ripples along the curves should be considered as noise. The step like structure around -12 eV is, however, real and caused by the two-dimensional singularities of a finite number of two-dimensional layers. These plots reveal a composite effect of bulk and surface properties. The fermi level for Ge lies around 0.4 eV and surface states are designated by A_1, A_2 and A_3. What we mean here by surface states are states which are very well localized on the surface. No distinction is made between bona fide surface states and strong resonances. Surface states A_1 are the usual states found in the fundamental gap and consist of two surface bands. These bands represent dangling bond states containing roughly 85% of the charge in the first layer. The states labelled A_2 and A_3 however are new but rather difficult to resolve. The A_2 states represent surface bond states which originate near the symmetry point M. They contain 86% of the charge in the first three layers. The states labelled A_3 occur mostly at and near the symmetry point $\bar{X}'$ but extend along $\bar{X}'$ to Γ and $\bar{X}'$ to $\bar{M}$. These states represent essentially s-like states at the surface with roughly 64% of the charge concentrated in the first layer.

For GaAs the fermi level lies near 0 eV and the surface states are labelled B_1, B_2, B_3 and B_1'. Surface bands B_1 and

B_1' are the usual bands obtained from a splitting of the A_1 bands caused by the differences in potential between the Ga and As atoms. In our calculations B_1 contains As dangling bond states with approximately 80% of the charge localized in the first layer. On the other hand B_1' contains mostly Ga dangling bond states with about 80% of the charge concentrated in the first layer. The surface states B_2 are new and have also been obtained using a different method [5]. These surface states are found mostly around $\bar{M}$. They represent GaAs bond states along the surface with roughly 80% of the charge in the first layer. Finally the most interesting new states are the B_3 states. These are surface states that exist near the lower energy band edge of the "heteropolar" gap and extend around 0.2 eV into this "forbidden" gap. They represent As s-like surface states with roughly 70% of the charge concentrated in the first layer. These states remain extended into the gap with small changes in the parameters. They appear to be an intrinsic property of As atoms on a surface. A further study of these states is in progress.

References

* Research supported in part by the National Science Foundation Grant No. GH35688, and the U.S. Atomic Energy Commission

† Present address: Department of Physics, MIT, Cambridge, Mass.

1. J. D. Joannopoulos and M. L. Cohen, to be published.
2. K. Hirabayashi, J. Phys. Soc. Japan 27, 1475 (1969).
3. K. C. Pandey and J. C. Phillips, Solid State Comm. 14, 439 (1974).
4. D. J. Chadi and M. L. Cohen, to be published.
5. N. Garcia, J. Solana and N. Cabrera, to be published.

Figure Caption

Figure 1. Total density of states of twelve (110) layers of Ge (a) and GaAs (b). The surface layers are taken to be unrelaxed. The important surface states are labelled A and B for Ge and GaAs respectively. A_1, A_2, B_1 and B_2 are new surface states obtained in these calculations and are discussed in the text.

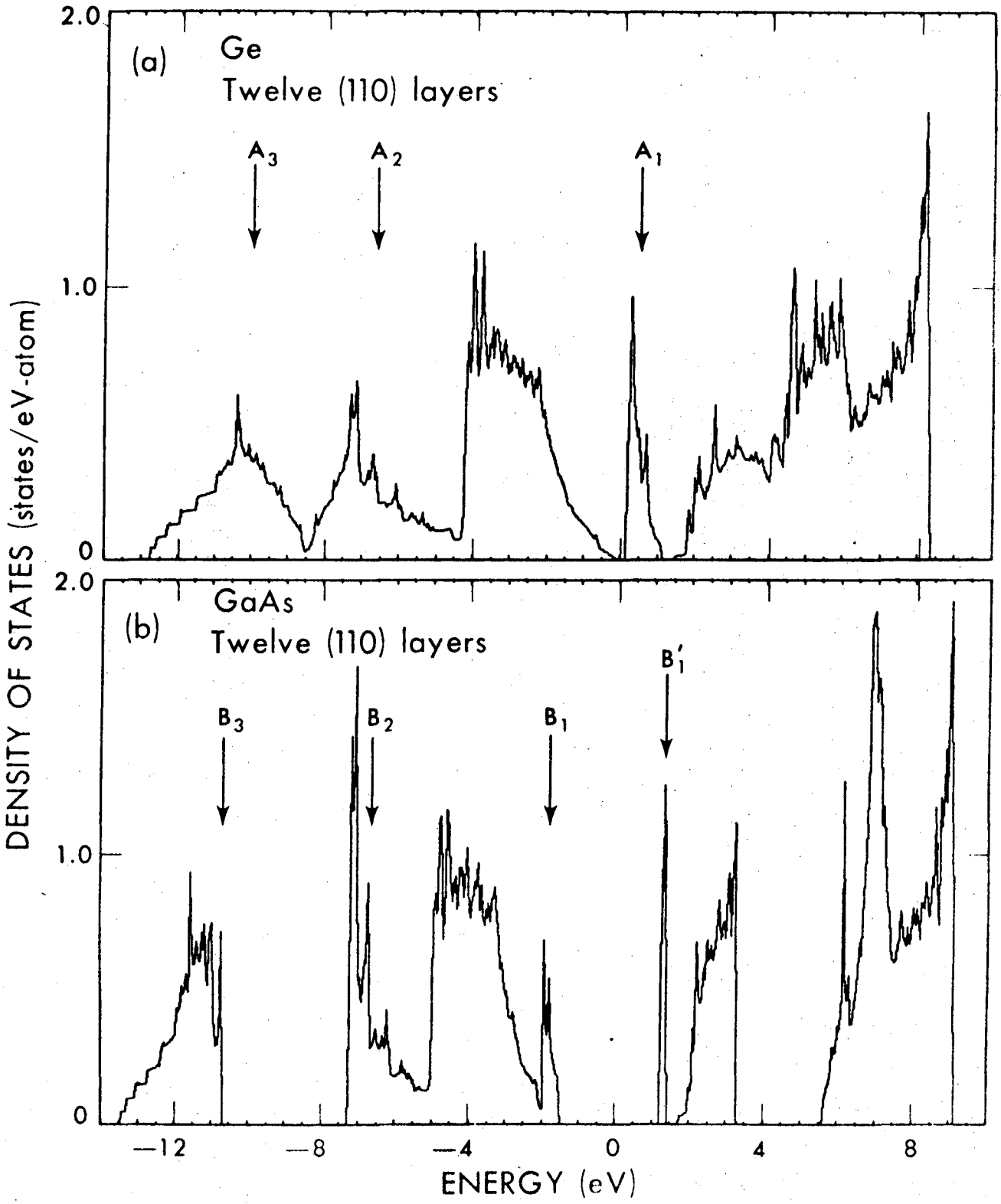

(a)
Ge
Twelve (110) layers
A3
A2
A1
(b)
GaAs
Twelve (110) layers
B3
B2
B1
B1'
DENSITY OF STATES (states/eV-atom)
2.0
1.0
0
—12
—8
—4
0
4
8
ENERGY (eV)

Fig. 1

TECHNICAL INFORMATION DIVISION
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720