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BOND CHARACTER AT A SILICON/COPPER SURFACE(U)
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C H PATTERSON ET AL. DEC 86 TR-2 N00014-86-K-0304

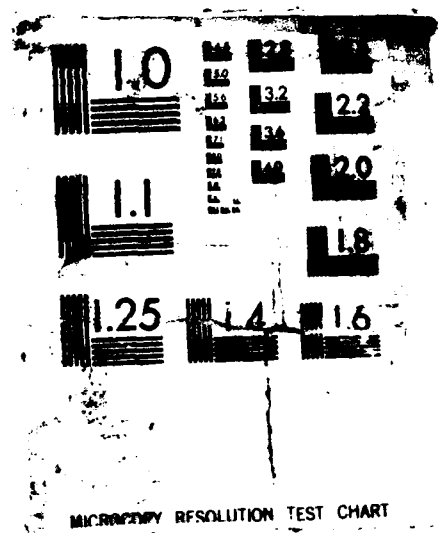
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Bond Character at a Silicon/Copper Surface

by

C.H. Patterson, E.W. Plummer, and Richard P. Messmer

Abstract Submitted

for the March 1987 Meeting of the

American Physical Society

University of Pennsylvania
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Abstract Submitted
for the March Meeting of the
American Physical Society
New York, NY
16-20 March 1987

Suggested Session Title:
23g, Surfaces, Semiconductors

Bond Character at a Silicon/Copper Surface. C.H. PATTERSON, E.W. PLUMMER and R.P. MESSMER, University of Pennsylvania. The ionic and covalent character of bonding is considered for the Si(111)-(5x5)Cu phase formed when one monolayer of copper is deposited on Si(111)(7x7) and subsequently annealed to 600°C. Localized orbitals and ab initio calculations have been employed to evaluate total energies and types of bonding for Cu adsorbed in several different sites, including the structure proposed by Chambers et al (1) on the basis of their angle resolved Auger electron spectroscopy results. The relation between the bond character of this phase and its surface spectroscopic properties is discussed.

(1) S.A. Chambers, S.B. Anderson and J.H. Weaver, Phys. Rev. B32, 581 (1985).

Standard Session Preferred

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