Metal Adsorption and Thin Film Adhesion on Si(100)

The development of microelectronic device technology requires detailed knowledge of metal-semiconductor and semiconductor-semiconductor interface formation. The scaling of integrated circuit components into the deep sub-micron range for the development of Ultra-Large Scale Integrated (ULSI) devices places new demands on the metal / Si(100) contacts, whether rectifying or ohmic. Interfacial phenomena, such as chemical reactions, lattice mismatch causing strain induced defects, and mixing across the interface, significantly influence the device properties as the devices shrink [4-6]. The energetics of metal adsorption and thin film or compound formation are essential to a fundamental understanding of these phenomena, yet the direct measurements of metal adsorption energies and adhesion energies on Si(100) have never been made, and indirect measurements are extremely rare and impossible for most systems due to silicide formation before desorption. The development of future microelectronic and optoelectronic devices will require semiconductor-semiconductor heterojunctions as well. The adsorption on Si(100) of semiconductors like Ge and other species like Ga and As which make III-V semiconductor compounds are of fundamental interest in understanding the formation of semiconductor-semiconductor interfaces. Again, the energetics of adsorption, thin film growth or compound formation at the monolayer level are essentially unknown, but necessary to a fuller understanding of the atomic-level details of these processes.

We will measure the heats of adsorption, the adhesion energies, and the sticking probabilities as a function of coverage for the atomic deposition of several species onto the Si(100) surface. The atomic adsorbates to be studied (Ag, Co, Ge, As and Ga) are important in metal / Si interfaces and semiconductor / Si heterojunctions. (For simplicity here, we will refer to these species collectively as "metals", although not strictly true.) These experiments will provide a direct measurement of the strengths of interaction between the deposition metal and the Si(100) surface. By integrating the heat of adsorption through the multilayer regime the adhesion energy for the film will also be obtained. This is true whether or not there is an interfacial reaction, and whether the multilayer film ends up being a pure element or a compound or alloy with Si. This fundamental information about the energetic stabilities of the species produced will clarify the thermodynamic driving forces which determine adsorbate structure and thin film morphology, in addition to answering questions about the degree of kinetic or thermodynamic control that is dominating the growth processes. Lastly, these experiments will provide a new direction in single-crystal adsorption microcalorimetry by proving that the technique can be extended to the many important adsorbate and thin-film systems on Si(100). A further extension allows us to study systems wherein Chemical Vapor Deposition (CVD) is used to grow films on Si(100), by implementing a *molecular* beam instead of the *metal atom* beam currently used.

In state-of-the-art quantum mechanical calculations of metal adsorption and adhesion energies on solid surfaces, serious approximations must still be made [7-15]. Our experimental energies will serve also as benchmarks to help theorists decide which approximations are acceptable. This, in turn, will help theorists to have confidence in their methods when addressing more complex issues.

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