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EXPERIMENTAL VERIFICATION OF A CLASSICAL MODEL FOR GAS SCATTERING FROM CRYSTAL SURFACES

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The energy transfer that takes place between an incident gas atom and a surface is of interest to many fields of science. Several models based upon classical mechanics have been proposed to describe this energy transfer process and the resulting angular distribution of the scattered gas. The hard cube model[1,2] and its successor, the soft cube model,[3] have been qualitatively successful in predicting the spatial distribution of thermal energy rare-gas atomic beams scattered from crystal surfaces. Other formulations[4,5,6] have met with varying degrees of success in their attempts to reproduces the observed data. In general, however, those models that do not restrict the surface temperature to zero degrees Kelvin yield the best results.

Recently Busby, Haygood, and Link[7] have presented a classical mechanical theoretical model that includes an attractive square well potential in addition to the surface temperature. A Monte-Carlo calculation of the trajectories of the scattered gas atoms was carried out, since, unlike the hard-cube model, the many body interaction did not permit a closed form solution to the gas-surface interaction. Their model also allows for scattering from ordered crystal domains of hexagonal and square arrays that simulate well the surface structure

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used in most experimental studies of surface scattering. The calculations, however, have been restricted to a consideration of the scattering of atoms from their own crystal lattice, that is, scattering of atoms from surface atoms of identical atomic weight. The major conclusions of their calculations are: a) the angle of maximum reflected intensity is independent of the beam incidence angle, incident energy, and surface temperature, and b) the capture coefficient or condensation coefficient for the incident beam increases with decreasing angle of incidence (defined with respect to the surface normal where $\theta=0$). The computed trajectories compared well with the experimentally observed spatial distribution of Ar atomic beams scattered from solid Ar surfaces.[7]

We would like to report the results of scattering studies of CO molecular beams from CO chemisorbed on a (100) crystal face of platinum and of the scattering of acetylene molecular beams from acetylene that was chemisorbed on the (100) crystal face of platinum. We have measured the angular distribution of the scattered molecules as a function of incidence angle. The experimental conditions in our studies approximate well those that were the basis of the computations by Busby et al. (same molecular weight of colliding gas and surface atom). Using low-energy electron diffraction we have simultaneously monitored the surface structure of the chemisorbed gases (CO and C_2H_2). Both of these gases form ordered surface structures on platinum[8] but the largest fraction of the chemisorbed molecules are in small square domains that give rise to broad, low-intensity diffraction spots (again, the real surface structure is similar to that assumed in the scattering model by Busby et al.). The molecular beam apparatus used in these studies is described in detail elsewhere.[9] The angular distribution of the scattered

molecular beam was measured as a function of incidence angle using a quadrupole mass spectrometer that can be rotated in the incident plane about the single crystal sample. Both carbon monoxide and acetylene were adsorbed at a pressure of approximately 10^{-7} torr and a temperature of 300°K. Once the LEED pattern indicated the appearance of the surface structure characteristic of these adsorbed gases, the experiment commenced. Figure 1 shows the spatial distribution of CO scattered from the CO-covered platinum (100) surface at various angles of incidence and at 300°K surface temperature. Figure 2 shows a similar plot for C_2H_2 scattered from adsorbed C_2H_2. For both gas-surface systems, the spatial distribution of the scattered beams appeared to be independent of the incident angle within the experimental accuracy. The scattered CO beam showed an intensity maximum between 30° and 40°, while the C_2H_2 beam appears to have a plateau in the range 10-40° scattering angle with respect to the surface normal.

An additional feature of the computed trajectories is that they are independent of the depth of attractive square well potential assumed operative between the incident gas and the surface. It is encouraging that molecules that are highly polarizable and have heats of sublimation different from that of Argon (1.8 kcal for CO and 5.1 kcal/mole for C_2H_2) obey well the spatial distribution characteristics predicted by the classical mechanical model. This agreement in the spatial scattering patterns of scattered molecules between experiment and theory indicates that the calculation realistically describes the non-reactive scattering of molecules from their own lattice and that the model may be used with some confidence to describe the scattering of molecules of various size

and chemical properties (polarizability, dipole moment, symmetry) from crystal surfaces.

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FIGURE CAPTIONS

Fig. 1. CO beam scattering as a function of incident angle from CO adsorbed on a Pt(100) surface. Surface temperature 300°K. The dotted line is drawn through the mean of all data.

Fig. 2. C_2H_2 beam scattering as a function of incident angle from C_2H_2 adsorbed on a Pt(100) surface. Surface temperature 300°K. The dotted line is drawn through the mean of all data.

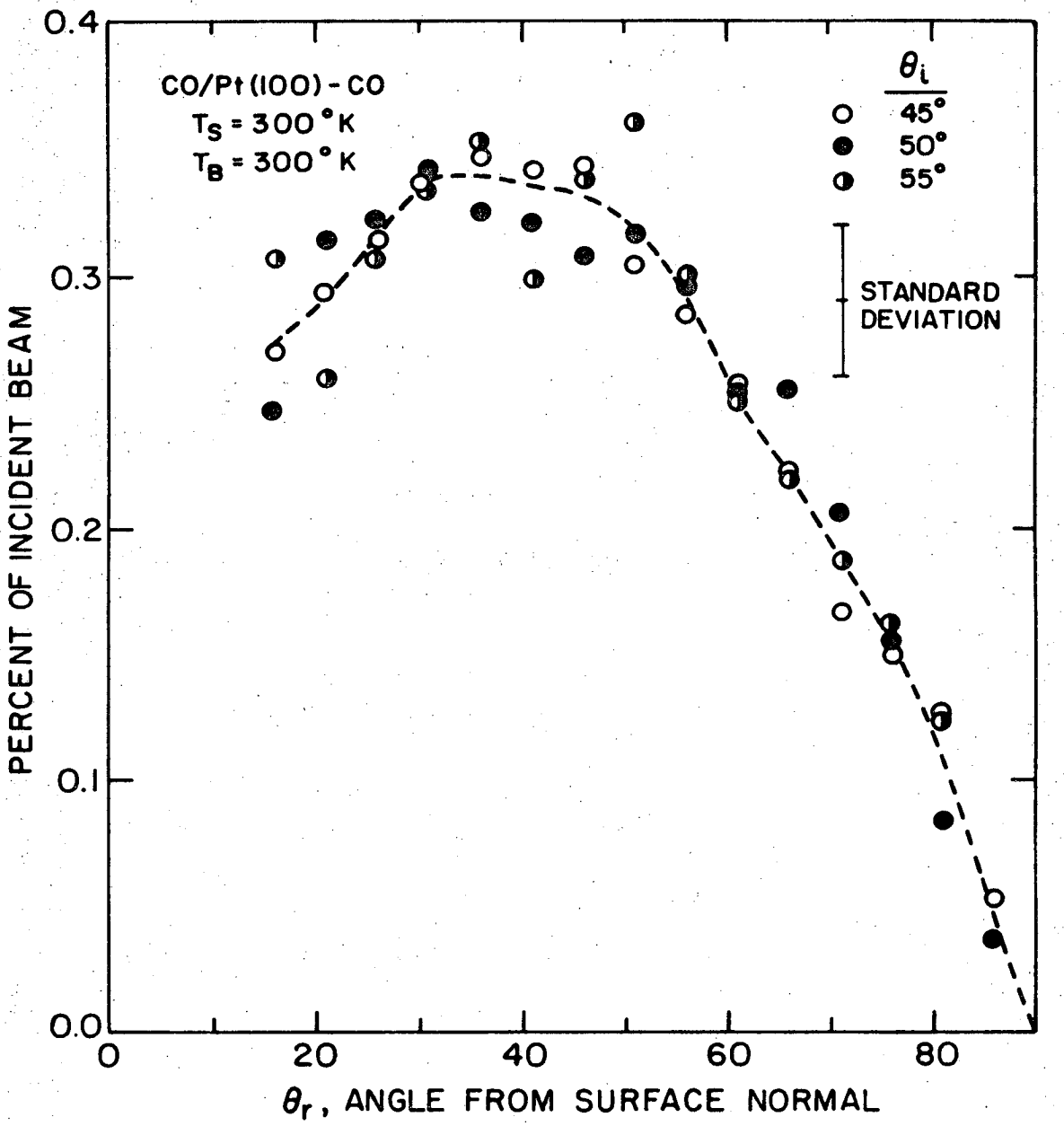

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Fig. 1.

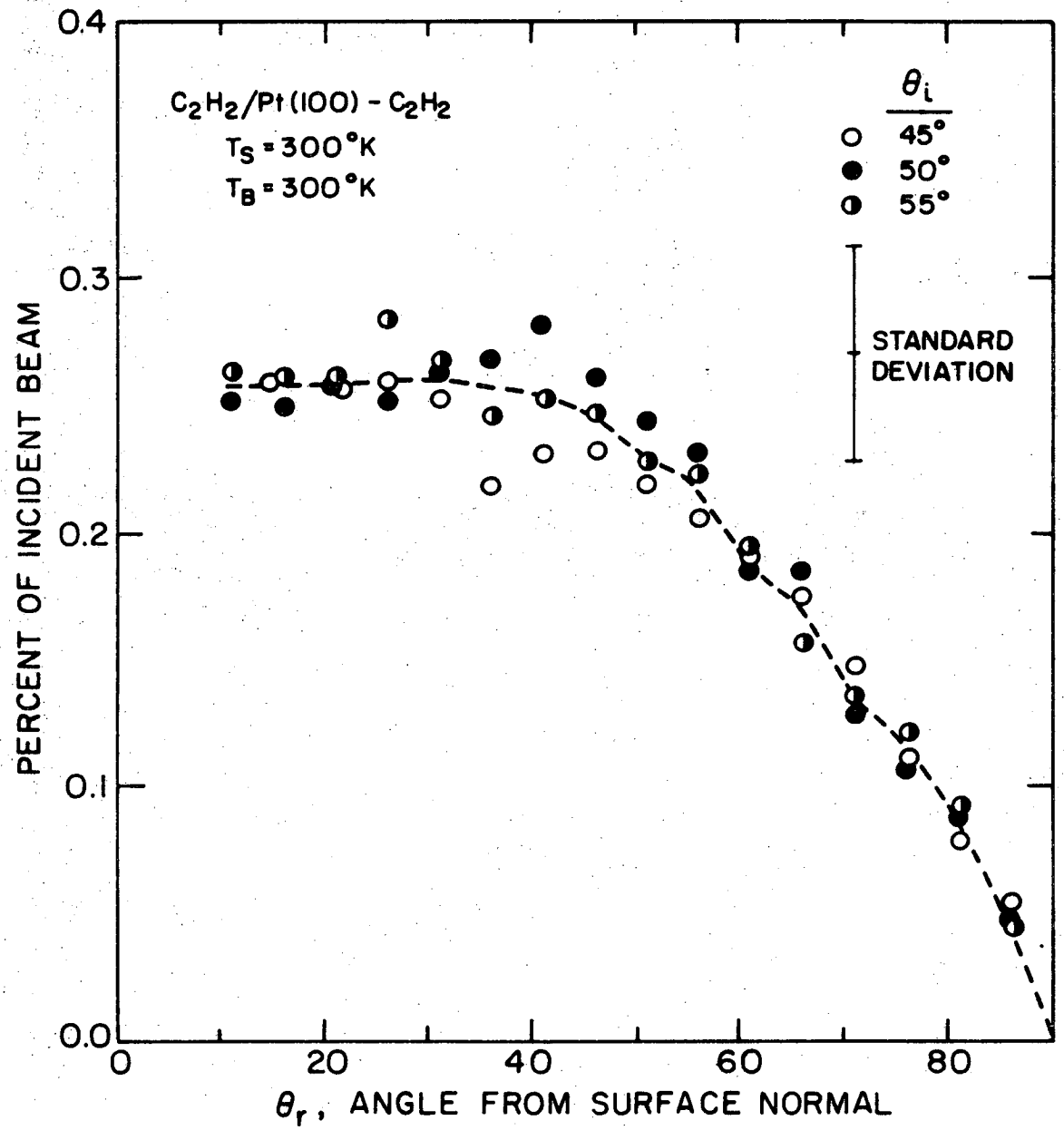

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Fig. 2.

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