Theoretical study of Nitrogen Scattering on W(100) Surface

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Résumé

The dynamics of nitrogen scattering from a W(100) surface is investigated by quasi-classical trajectory simulations in order to rationalize the measured scattered angle dsitributions (C.T. Rettner et al., J. Chem. Phys **93** (1990) 1442). The evolution of the width of the angular distributions is found non-monotonic with the translation energy of the impinging N2 molecules. After a description of the theoretical model, an original interpretation is prosposed for this rather puzzling behaviour. The shape and position of the angular distributions as well as the final translation energy distribution of the scattered nitrogen molecules are discussed.

Mots-Clés: reaction dynamics, heterogeneous processes, gas, solid interface.

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