Gross and Scheffler Reply: Among other things (e.g. steering and steric effects in dissociative adsorption) we had predicted [1] that the initial sticking probability of H_2 molecules impinging at clean Pd (100) exhibits oscillations, reflecting the quantum nature of the scattering process. In the preceding comment Rettner and Auerbach (RA) analyze experimental results and conclude that these oscillations are not detectable and thus either not existing or at least very small.

In this reply we argue that the experimental study of RA is not conclusive to rule out the existence of quantum oscillations in the scattering of H_2 and note several problems and incongruities in their study:

1) In their figure RA compare measurements at an angle of incidence $\theta_i = 15°$ to our calculations performed for normal-incidence, i.e. $\theta_i = 0°$ [1].
2) RA argue in their analysis that substrate vibrations can be treated in a "surface mass model".
3) The experimental intensity of reflected H_2 molecules was integrated over a large angle.

We now elaborate on these points and explain some aspects which show that the measurement of the predicted quantum oscillations is a most challenging project.

1) Angle of incidence – The oscillatory structure of the sticking probability is a consequence of the quantum nature of H_2 scattering and reflects the opening of new scattering channels and resonances with increasing kinetic energy. In a simplified description, i.e. neglecting rotational and vibrational degrees of freedom of H_2, elastic scattering gives rise to reflected beams: $|(\mathbf{k}_\parallel + \mathbf{g}), -\sqrt{k_z^2 - 2\mathbf{k}_\parallel \cdot \mathbf{g} - \mathbf{g}^2}\ \rangle$. Here $(\mathbf{k}_\parallel, k_z)$ is the wave vector of the incident H_2 beam and $\mathbf{g}$ is a two-dimensional reciprocal lattice vector of the surface. The condition for emerging beams is that the argument under the square root is positive. Just before a new beam can emerge, it is already built up though it remains confined to the surface. Thus, this beam can not (yet) be observed directly, but as it is coherent with the other beams these other will exhibit sharp resonance structures. Furthermore, oscillations could be caused by selective adsorption resonances [2]. If there are many scattering states, the effect will be small, because it will be distributed over all states.

Hence the strengths and energies of the oscillatory structures depend sensitively on the initial conditions. A general angle of incidence has disadvantages because the number of symmetrically distinct states is larger than for normal incidence. For an incident angle of $\theta_i = 15°$ the oscillations are therefore much shallower compared to the normal-incidence results, as confirmed by recent calculations that we have performed. – These effects are well known from other quantum-mechanical scattering studies, e.g. in low energy electron diffraction (see, e.g. Ref. [3,4]).

2) Influence of substrate vibrations – As discussed under item 1, the oscillatory effects are due to molecules which occupy beams which are still trapped at the surface, i.e. which are bouncing back and forth between the substrate and the energy barrier towards the vacuum. This dynamical trapping will lead to a much larger influence of the substrate vibrations than considered in the "surface mass model", which simply averages over incident velocities. In fact, not the phonon energies are expected to cause the main problem, but the loss of coherence of the temporarily trapped hydrogen.

3) Integrating over all directions – Such integration typically obstructs the observation of quantum oscillations because it also considers all incoherently scattered molecules. In fact, for a slightly imperfect Pd (100) surface it is likely that most molecules are reflected into "inelastic directions" $(\mathbf{k}_\parallel + \mathbf{g} + \mathbf{q})$, where $\mathbf{q}$ is a wave vector describing the interaction with a phonon or with a surface imperfection. The sticking probability of H_2 at small kinetic energies of ≤ 0.05 eV is rather large ($\approx 60\%$). This leads very rapidly to the adsorption of some hydrogen during scattering experiments, a particularly strong effect at low surface temperatures as used by RA. From the above discussion it can be inferred that the oscillatory structure is particularly sensitive to the surface potential, and even a small number of adatoms and other surface imperfections (e.g. steps) will reduce the scattering coherence. As coherence is lost, these molecules will not contribute to the oscillatory behavior. – These incoherence effects will be largely filtered out if only well defined quantum states, which are consistent with elastic scattering, e.g. one reflected beam, were measured. We therefore suggest to monitor only *diffraction* intensities and not the whole reflection flux in order to resolve an oscillatory structure.

In conclusion, we are convinced that the quantum mechanical resonance structures of H_2 dissociation and scattering do exist, but the experimental detection certainly requires particular care. Under appropriate experimental conditions the predicted oscillations will be observable, as they have been found in He and H_2 scattering since the 1930s [2] and in electron scattering [3,4].

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