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Comment on "density functional simulation of a breaking nanowire" Nakamura et al. reply

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Nakamura *et al.* Reply: Stafford, Bürki, and Baeriswyl [1] (SBB) raise in a Comment to our Letter [2] the important question, Is the atomistic first principles simulation *realistic*—“i.e., whether it can be compared to experimental results [3] obtained for a single nanocontact between two macroscopic pieces of metal”? We employ for technical reasons periodic boundary conditions in our density-functional simulation, i.e., we consider an infinite wire with a periodic modulation in width along the wire. The authors question the convergence in unit cell size of the calculated force in our simulation.

Density-functional-theory (DFT) calculations are often restricted to small system sizes due to limitations in computer time and memory, and our simulation is no exception to that. So, in principle, therefore we cannot disagree with the authors of the Comment that it could be worthwhile to do calculations on larger systems in order to check boundary effects due to quantum interference (and other effects). However, it should be pointed out that a direct check for size effects in the type of simulation we performed is not simple since the evolution of a particular contact depends rather sensitively on the detailed initial configuration. Thus the atomistic simulations have a stochastic nature, just as the experiments.

SBB base their criticism on a model consisting of two serially connected constrictions with hard-wall boundaries in a free-electron gas. For this particular model they find a correction due to quantum interference between the two contacts which gives rise to significant change in the cohesive force in their model. We find this model of cohesion very simplified and it is not obvious at all that their results can be directly compared with ours (also their calculation does not in fact involve periodic boundary conditions).

Let us point out some of the essential differences between our calculations and the hard-wall model used by SBB. Firstly, in our calculations the structure develops self-consistently both with respect to the ionic and electronic degrees of freedom, i.e., the ions are allowed to move to their relaxed equilibrium positions and the electron density can readjust and screen changes in the electronic potential. One consequence of the ionic motion is the appearance of sudden structural changes associated with atomic rearrangements. These effects are not treated at all in the hard-wall model, where the shape of the contact is externally controlled and where electronic screening is ignored. Secondly, the energy and force in our simulation comes from complete DFT calculations involving kinetic, electrostatic, and exchange-correlation contributions. The hard-wall model uses only an electronic “band” term. Thirdly, we use a realistic self-consistently deter-

mined scattering potential which includes ionic scattering and surface corrugation. The nonadiabaticity of the potential gives, for example, rise to the calculated deviations from the $3G_0$ plateau. In contrast, the hard-wall model has a flat potential with an adiabatic, smoothly varying hard-wall confinement.

The severe shortcomings of the hard-wall model (no corrugation, no self-consistency, no screening, only band energy), especially the idealized scattering conditions, will certainly emphasize electronic shell and interference effects and it is therefore not clear that the estimates presented by SBB can really be applied to our simulation. If we, for example, consider the regime of cell lengths in our calculation larger than, say, 24 \AA , we find the force to be constantly between 0.1 and 0.3 nN in the whole range until the wire breaks. From the hard-wall model the force fluctuations in the same regime should be about 0.6 nN.

In conclusion, we do not think that the hard-wall model presented by SBB can be used to answer the question of possible interference effects for contacts with real atomic structures. But, on the other hand, we basically agree with SBB that it could be worthwhile to perform larger-scale density-functional simulations in order to ensure that interference effects do not play a role.

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- [3] G. Rubio, N. Agrait, and S. Vieira, Phys. Rev. Lett. **76**, 2302 (1996); A. Stalder and U. Dürig, Appl. Phys. Lett. **68**, 637 (1996). [We note that these articles referred to by SBB describe measurements of the cohesive force in gold nanocontacts. Our calculations were performed for sodium contacts for which no force measurements, to our knowledge, have been performed. For conductance measurements of sodium nanocontacts we refer to J. M. Krasns *et al.*, Nature (London) **375**, 767 (1995)].