Ab-initio study on scattering potentials of defects on Ge(001) surfaces

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INTRODUCTION

As new techniques for the nanoscale manipulation and modification of materials progress, the electron scattering properties of nanostructures are the focus of attention both experimentally and theoretically. Although scanning tunneling microscopy and mechanically controllable break junctions have been used to examine the scattering properties of nanoscale systems sandwiched between two electrodes, it is not easy to discuss the contribution of local chemical bonds to the electron scattering using these techniques. On the other hand, the spatial maps of the local density of states obtained by scanning tunneling spectroscopy can give us the images of standing waves, which provide important information about the dispersion relation of the electron scattering process at the potential barrier.

COMPUTATIONAL METHODS AND MODELS

I carried out first-principles calculation for obtaining the scattering potential of the defects on Ge(001) surfaces using a computational model shown in Fig. 1 [1]. The Ge-Ge dimer at the center of the scattering region is replaced by Ge-Si or Ge-Sn dimer as a defect. When the Si and Ge atoms are located at the lower and upper sides of the dimer, respectively, the dimer is referred as an SiL dimer. Other dimers are named in a similar manner. By calculating the scattering wave functions using the overbridging boundary-matching method [2], the standing waves in the spatial map of the local density of states are examined; the waves correspond to the image of the differential conductance obtained by scanning tunneling spectroscopy [3].

DISCUSSION

The charge density distribution of the scattering wave functions for the electrons propagating from both the left and right electrodes is investigated with an energy of E_F+0.55 eV, which corresponds to the spatial image of the differential conductance in the scanning tunneling spectroscopy spectrum [3]. The line profiles of the standing waves along the dimer row including the impurity atom are depicted in Fig. 2. It should be noted that the charge density of the π^* band above the lower atom of the dimer is larger than that above the upper atom. To demonstrate the period and phase shift of the standing waves clearly, the density of the standing waves is fitted by

$$\alpha(x) = \mathrm{A}\cos(2k_x x + \varphi) \quad (1)$$

where A, φ, and k_x are the amplitude of the standing waves, phase shift of the standing waves, and Bloch vector in x direction, respectively. The fitting is carried out using the density of the standing waves above the lower atoms of the dimers, which are indicated by closed circles in Fig. 2.

The period of the standing wave and its phase shift are shown in Table I, in which they agree with those obtained by the experiment [3]. The scattering potential acts as a barrier when the electronegativity of the upper atom of the dimer is larger than that of the lower atom, while it becomes a well in the opposite case. The scattering potential is related to the stabilization of the π bands of the Ge(001) surface due to the difference in electronegativity between Ge and the impurity.

CONCLUSION

The scattering potential of the defects on Ge(001) surface is investigated by first-principles

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calculation. The phase shifts of the standing waves due to the defects are in agreement with those obtained by experiments [3]. By calculating the reflection coefficients of the scattering wave functions, it was found that the scattering potentials of the SiL and SnU dimers act as a well, while those of the SiU and SnL dimers behave as a barrier. This characteristic is interpreted in terms of the electronegativity of the defects; when the electronegativity of the upper site of the dimer is large, the energy gap between the π and π^* bands increases, resulting in the generation of the potential barrier for the π^* electrons.

REFERENCES

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Table I. Amplitude and phase shift of the standing waves around the Ge-Si and Ge-Sn dimers.

	Model			
	SiL	SiU	SnL	SnU
Amplitude (10^{-7}e/Å^3/eV/spin)	3.908	1.692	7.169	1.031
Phase shift (π rad)	0.221	-0.602	-0.650	0.142

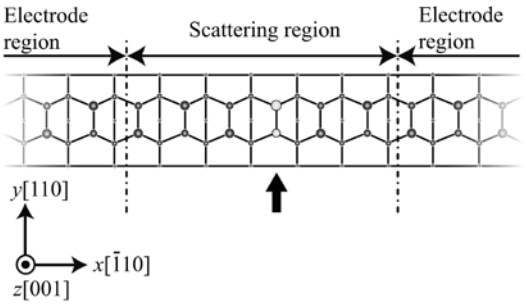

Fig. 1. Schematic image of computational model. Dark spheres are Ge atoms and light spheres represent the dimer replaced by a Ge-Si or Ge-Sn dimer, which is indicated by the arrow. Atoms are denoted by large and small spheres according to the distance from the surface. Reprinted from Ref. 1.

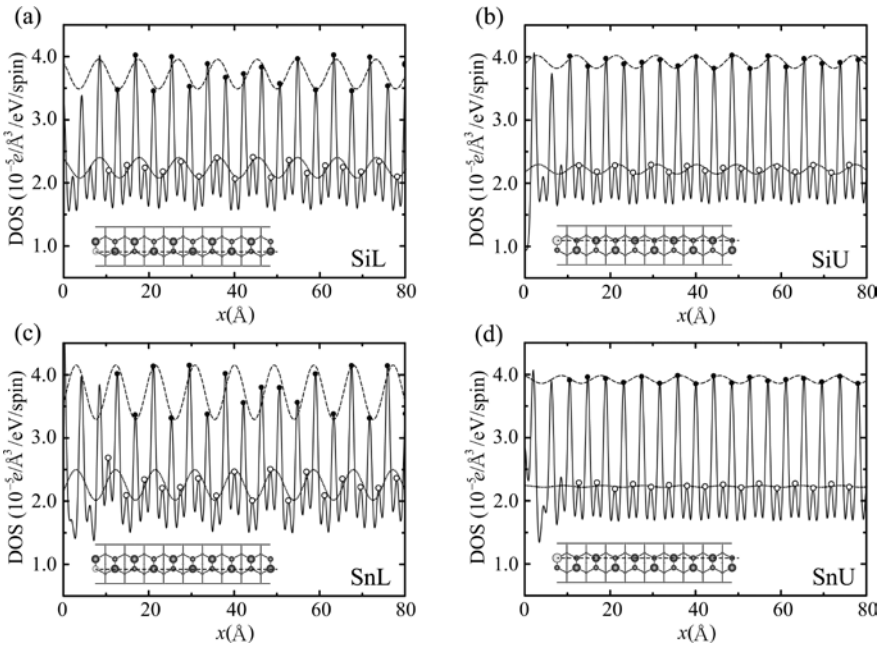

Fig. 2. Line profiles along dimer row including impurity atom indicated by dashed lines in insertions, where the meanings of symbols are the same as those in Fig. 1. Solid curve represents the standing wave. Dashed and dotted curves are fitted by Eq.~(1) using the densities above lower atoms of impurity side (closed circle) and upper atoms of impurity side (open circle), respectively. Reprinted from Ref. 1.