ABSTRACT OR SUPPORTING INFORMATION

1. Title of article
Substrate Effects on Electronic Properties of Atomic Chains

2. Author of article
Toshishige Yamada (phone: 4-4333, email: yamada@nas.nasa.gov)

3. Submission of article
This will be submitted to the 1998 Foresight Conference, Santa Clara, CA, on November 12-15, 1998. The Program Committee will screen these submitted articles and select works that are of good scientific quality. Only those selected are entitled to present in a conference (either a talk or a poster) and write a full paper in a journal. Thus, a paper has not been written yet. They will notify us the result in a couple of months. A paper will be written after accepted, and another form1676 will be filed at that time.

4. First appearance of article
When accepted, this article, with all accepted other articles, will be posted on a web site, http://www.foresight.org/conference/MNT6/index.html near the conference dates of November, 1998.

5. About VI author/originator verification in form1676
There is no export controlled, confidential commercial information. Regarding a patent, this belongs to the same field as my invention disclosure I filed in April 1998 at NASA Ames.
(a) In April, 1998, I had filed an invention disclosure "Doping method of semiconducting atomic chains at NASA Ames, and it was submitted to the U.S. patent office in early June, 1998.
(b) This article itself cannot be another invention disclosure, since it is so concisely written that it is impossible to extract a patentable idea. In filing a patent, scientific quantities (such as an electron energy) to specify the idea are essential, but there is little such description. Figure 1 is a theoretical plot to mathematically show the existence of the edge state. There are no experimental data.

6. Article
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When the device size is reduced down to 0.07 micrometers, the number of dopant atoms in the channel will no longer be macroscopic, typically less than a hundred. A spatial distribution of these dopant atoms will fluctuate statistically from device to device even in identically designed devices, and this places a serious limitation for integration. It is, however, impractical to control dopant positions within atomic dimension. One fundamental solution to this problem is to create electronics with atomically precise, but preferably simple structures. Atomic chains, precise structures of adatoms created on an atomically regulated surface, are candidates for constituent components in future electronics. All the adatoms will be placed at designated positions on the substrate, and all the device structures will be precise, free from any deviations. It was predicted using the tight-binding calculation with universal parameters (Harrison, 1980) that silicon chains were metallic and magnesium chains were semiconducting regardless of the lattice spacing (Yamada et al., 1996), and a possible doping method was also proposed (Yamada, 1998). In these treatments, the substrate was assumed to serve as a non-interacting template holding the adatoms without a formation of chemical bonding with substrate atoms. However, this scheme may not be easy to implement experimentally. Adatoms will have to be fixed with a van der Waals force on the substrate, but the force is generally weak and an extremely low temperature environment has to be prepared to suppress their unwanted thermal displacement. It may be logical to seek a scheme to allow the adatoms to form chemical bonding with the substrate atoms and secure their positions. The substrate effects are studied in detail.

Once chemical bonds are formed, there is no guarantee that electrons are confined within the adatom system. In the worst scenario, the independent adatom structures will interact strongly through an overlap of wave functions inside the substrate, resulting in large crosstalk. This is not appropriate in device applications and must be avoided. A tight-binding consideration shows that if the substrate is made of crystals with a natural lattice spacing shorter than the s-p crossing point, dangling bonds of substrate atoms cannot penetrate into the bulk, and

automatically localize at the surface. Examples for this type of substrate is a usual silicon crystal, a germanium crystal, a galium arsenide crystal, and many metallic crystals like copper. Oppositely, if the lattice spacing is longer than the s-p crossing point, then there are no such surface states, and all the modes penetrate deep into the substrate. Examples are alkali halide crystals, like sodium chrolide. Apparently, we need to stick to the former s-p crossing substrate as long as the chemical bonding scheme is sought.

Figure 1(a) shows the energy levels of a one-dimensional chain created with 24 silicon atoms having an s-orbital and a p-orbital each, imagining that the spacing can be changed as a gedanken experiment (in reality, there is one preferred spacing minimizing the system total energy) using the same tight-binding method. This is a mathematically simplified one-dimensional model, and surface states correspond to edge states, where electrons strongly localize at the dangling bonds of edge atoms. The figure shows that the edge states always appear in the middle of the band gap once after the s-p crossing has occurred. Figure 1(b) is the electron existence probability at the edge atoms, and it is clearly seen that the electron wave function for these modes localize more strongly for shorter spacing. The edge states are quite rebust, and their existence is not influenced by the detail of the lattice symmetry.

It is also shown that such edge states are eliminated when the dangling bonds are saturated with hydrogen atoms n the same crystal. This is because the participation of s- and p-orbitals are essential for the formation of edge states after the s-p crossing, while p-orbitals are irrelevant in a hydrogen atom. We can use hydrogen atoms as if they were insulation materials. This is true regardless of the crystal orientation of the surface as long as an s-p crossing crystal is used. The idea of using hydrogen atoms is not new (Watanabe et al 1996), but a relation of a free dangling bond and a hydrogen terminated dangling bond has not been discussed in the context of changing the lattice spacing from infinity.

The chemical bonding has two major effects on the chain electronic properties. First, only the remaining s- and p-orbitals not used for the chemical bonding can decide the chain band properties, rather than the full set of orbitals previously assumed. In fact, when two orbitals form a chemical bond, there appear bonding and antibonding states, separated by double the covalent energy, which is usually on the order of several electron volts. Two electrons, one of which is from the adatom and the other from the substrate atom, will occupy the bonding state and form a covalent bond, possessing much lower energy than the original. As a result, they cannot contribute to the chain properties, and one electron in the adatom is effectively eliminated per chemical bond. Second, because of a possible HOMO energy difference between an adatom and a substrate atom, semiconducting chains are unintentionally doped. These effects are studied with a self-consistent tight-binding method with universal parameters (Harrison and Klepeis 1988). With one adatom per unit cell, adatom chains are semiconducting (1) if adatoms are of group III and form one chemical bond per adatom, or (2) if adatoms are of group IV and form two chemical bonds. The previous result of realizing semiconducting chains by group II adatoms without chemical bonds is consistent with this picture. When the HOMO energy in an adatom is shallower than that in a substrate atom, the entire chain is positively polarized, unintentionally achieving p-type doping. When deeper, the chain is negatively charged, achieving n-type doping. A substrate significantly changes the electronic properties of the adatom chains and the careful considerations are needed for electronics applications.

References

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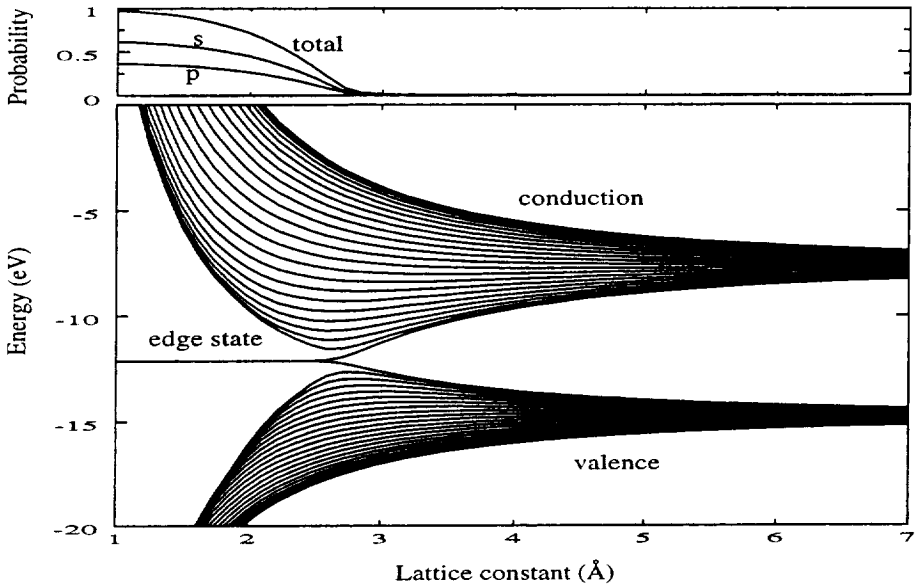

Fig. 1. (a) Energy states of a chain with 24 silicon atoms and (b) electron existence probability at the edge atoms as a function of lattice spacing.

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