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Electronic Structures of Si-Based Man-Made Crystals

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Electronic structures have been calculated for Si-based manmade crystals by using a tight-binding sp^3s^* model with homogeneous strain. Interesting properties, such as direct transition and pseudo narrow-bandgap, appear especially in the crystals where two mono-layers of non-Si atoms are stacked along the (111) orientation.

§1. Introduction

Much interest has been paid recently to manmade crystals where more than two different kinds of atoms are artificially aligned. Si-based manmade crystals are especially interesting since they will give a breakthrough in physical limits given to the present VLSIs.

Effective-mass approximation based on the free-electron image is commonly used in analyzing superlattices [1,2] This model is, however, insufficient for the theoretical analysis of the manmade crystals. It is the essential demand to take directly the effects of mutual coupling between different kinds of atoms into account, and only this can predict unique properties of the manmade crystals. In this paper, we have analyzed the Si-based manmade crystals by using a tight-binding model.

§2. Electronic structures of bulk Si and Ge

The sp^3s^* nearest-neighbor semi-empirical tight binding model [3] can represent well electronic structure of indirect semiconductors such as Si and Ge. Values of parameters of Si, Ge and P atoms used in this work are taken from ref.[3]. Interatomic matrix element among the different kinds of atoms is assumed to have an averaged value of the corresponding matrix element [4]. Harrison's bond orbital model [5] is used as the valence band discontinuity.

In case of Ge, electrons at the conduction band edge are in the s-s anti-bonding orbit at the Γ point (k=0). With increasing k from zero, a part of electrons enter into both p and excited s, i.e., s^* orbits to couple with those of the adjacent lattice plane of atoms. Phase of the three orbits, i.e., the phase of envelope-function advances in proportion to k, which can be interpreted as free electrons in the extended states.

At the X point, the phase difference θ becomes 90° between the adjacent lattice planes. Situation at the L point is perfectly different from that at the X point although the average θ value takes also 90°, as shown in Fig.1. This is caused by the fact that there are two different spaces between the lattice planes, namely, short space A_S and long space A_L, along the L orientation. Since there are three times more bonds between the adjacent lattice planes across A_S than those across A_L, there is no phase difference at A_S. That is, electrons are predominantly in the s-s and p-p anti-bonding orbits even at the L point. The phase is then rotated by 180° between the adjacent lattice planes across the space A_L, where electrons are in the s-s and p-p bonding orbits.

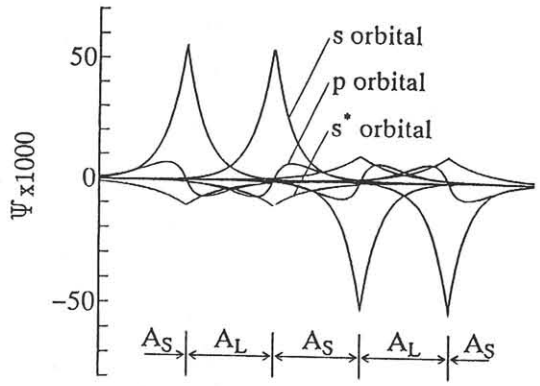

Fig.1 Schematic wavefunction of bulk Ge at the L point along the bonds.

The similar situation can be observed in Si when we exchange the s orbit to the p orbit, and vise versa. This is because, in case of Si, electrons in the p-p anti-bonding orbit have lower energy than those in the s-s anti-bonding orbit.

§3. Classification of basic manmade crystals

Si-Ge manmade crystals having the same number of Si and Ge atoms can be classified into four types as shown in Fig.2, from a view point of number of

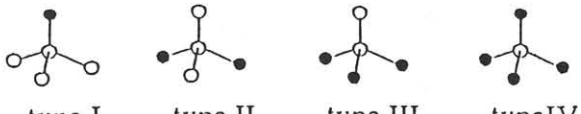

Fig.2 Bonding types of the manmade crystals.

neighboring Ge (or Si) atoms bonded covalently with an Si (or Ge) atom at the center.

The type–I is the most interesting where the center atom has only one atom of a different kind among its four neighboring atoms. Original properties of Si–Si and Ge–Ge bonds are most strongly remained in a polarized form.

Precisely speaking, the type–I crystal can be divided into two crystal structures. The first is of Si_2Ge_2 aligned along the (110) orientation, and the second along the (111) orientation as shown Fig.2, if we apply the notation commonly used in the superlattice. We will discuss only on the second crystal. In this crystal, the lattice planes of the same kind of atoms are at A_S but these of another kind of atoms at A_L. There is the type–III Si_2Ge_2 crystal aligned along (111) orientation, whose lattice planes of the same kind of atoms are at A_L. It was found that this type–III crystal has no interesting properties and thus we do not discuss here.

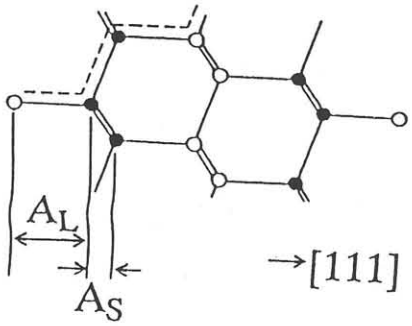

Fig.3 Structure of the type–I Si–Ge manmade crystal aligned along (111) orientation.

§4. Electronic structure of the type I crystal

Electronic structure is shown in Fig.4. The bond length is assumed equal to that (=2.39Å) of the free standing SiGe crystal. Valence bandedge of Si is taken as an origin of energy (E=0). The electronic structure is very near the direct transition type where energy takes the minimum value in the conduction band at the Γ point. This origin can be clearly understood from wavefunction at the Γ point schematically shown in Fig.5.

Due to the zone–folding effect, characteristics of bulk Si and Ge at the L point are reflected to those at the Γ point. Electrons at the Ge–Ge bond are predominantly in the s–s anti–bonding orbit as those in A_S of bulk Ge at the L point, while electrons at the Si–Si bond are predominantly in the p–p anti–bonding orbit as those in A_S of bulk Si. Transitions between these two polarized features occur at the Si–Ge bond, i.e., across A_L where number of bonds is a few. Density of electrons is high in the s–s orbit at the

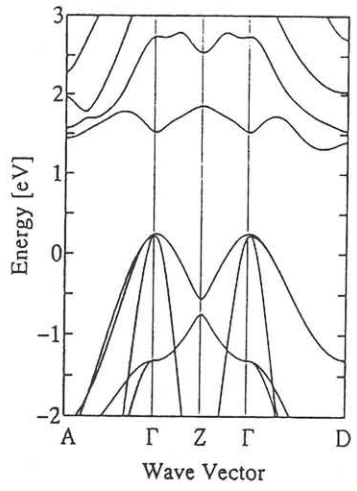

Fig.4 Electronic structure of the type–I Si–Ge manmade crystal under free standing condition.

Ge–Ge bond than in the p–p orbit at the Si–Si bond as clearly shown in the figure. Since electrons are accumulated at the Ge–Ge bond having the s–s anti–bonding like form as those in Ge at the Γ point, total energy is very near that of bulk Ge at the Γ point. Energy near the Γ point, however, is increased with k by the effect of the adjacent Si atoms.

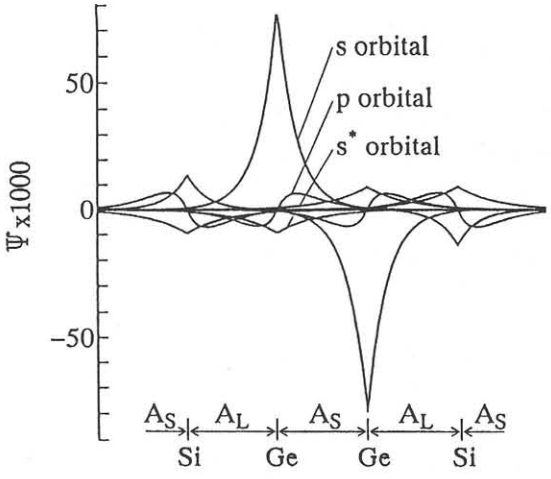

Fig.5 Schematic wavefunction of electrons at the Γ point of the type–I Si–Ge manmade crystal.

Coupling effects of electrons are decreased in inversely proportion to square of the bond length [5]. Thus energy at the Γ point is decreased with increasing the bond length. Energy except at the Γ point, however, is increased with the length. This is due to the reduced effects of the s^* orbit, which forms a strong s^*–p bonding and decreases the energy at large k. Thus, elongation of bond length to that (=2.45Å) of bulk Ge changes the manmade crystal to the direct transition type as shown in Fig.6.

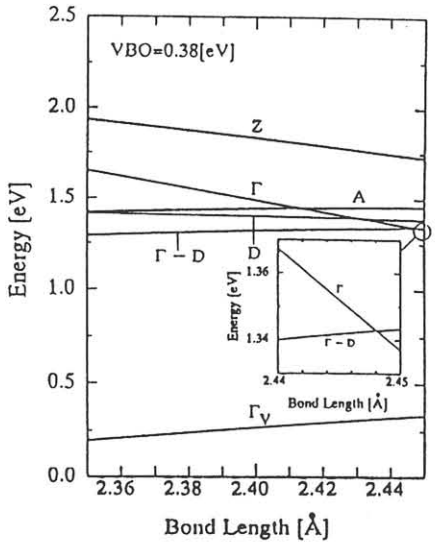

Fig.6 Energy as a function of bond length for the type-I Si-Ge manmade crystal.

§5. Electronic structures of Si-Ge-P manmade crystals

Electrons are still localized at the Ge-Ge bond having the s-s anti-bonding like form even when number of the lattice planes of Si atoms is increased from 2 to 2n in order to form the type-I like $Si_{2n}Ge_2$ manmade crystal. This fact means that when one of two lattice planes of Ge atoms is replaced to a plane of P atoms, electrons will be still localized strongly at the Ge-P bond, resulting in deep donor levels.

Electronic structure is shown in Fig.7 for the type-I like $Si_{14}Ge_1P_1$ manmade crystal. The minimum energy relating the Ge-P bond is about 0.25eV below the conduction bandedge. Since these deep levels are extended along the lattice planes of Ge and P atoms to form a band, but localized perpendicular to these the conduction bandedge, a pseudo narrow-gap semiconductor is newly formed with anisotropic transport properties where the deep band acts like a valence band.

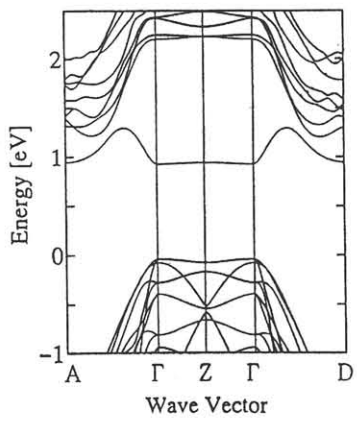

Fig.7 Electronic structure of the $Si_{14}Ge_1P_1$ manmade crystal.

Taking these features into consideration, a novel hetero-junction bipolar transistor (HBT) shown in Fig.8 has been proposed. Emitter and collector are of uniformly doped n type Si, while intrinsic base is of the n type Si-Ge-P manmade crystal. Low energy electrons at the deep level in the intrinsic base region are injected from the valence band in the extrinsic p-base region along the lattice planes of Ge and P atoms. High energy electrons injected from the emitter can jump over these ultra narrow planes, and reach the collector. Low turn-on voltage of about 0.2V is the most attractive feature of this HBT, which results in the small power-delay product.

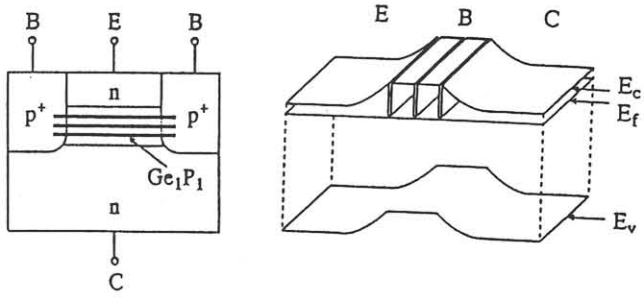

Fig.8 Schematics of proposed HBT with pseudo narrow bandgap manmade intrinsic base region.

§6. Conclusion

Novel properties have been predicted for the Si-based manmade crystals aligned along the (111) orientation. They will be very useful both to light emitting devices for optical interconnection and to low-power & high-speed LSIs.

It is worthy to make a final comment that there is an uniaxial strain in the interesting crystal, whose effects should be studied extensively.

References

[1] T.Ando et al.,: A Chapter in "Physics and Application of Semiconductor Superlattice" ed. by Physical Society of Japan (Baihukan, Tokyo, 1984).
[2] G.Bastard: Physical Rev., B25 (1982) 7584.
[3] P.Vogel et al.,: J. Phys. Chem. Solids, 44 (1983) 365.
[4] T.Saito et al.,: Superlattice and Microstructures, 9 (1991) 377.
[5] W.A. Harrison: "Electronic Structure and Properties of Solid", (Freeman, San Francisco, 1980).