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13. ABSTRACT *(Maximum 200 words)*

For the past several years there has been a major international effort [1–4] on the heteroepitaxial growth of compound tetrahedrally coordinated semiconductors on Si substrates by MBE, MOCVD, etc.; on the fabrication of devices and circuits in these layers; and on the monolithic integration of such components with Si circuits fabricated on the same wafer. This effort is based on the significant potential that epitaxial growth of dissimilar semiconductor materials holds for technological applications. Nevertheless, relatively little theoretical work has been performed to understand the fundamental interactions and global issues governing the initial stages of growth and the structure of the first few mono-layers in these systems.

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For the past several years there has been a major international effort [1–4] on the heteroepitaxial growth of compound tetrahedrally coordinated semiconductors on Si substrates by MBE, MOCVD, etc.; on the fabrication of devices and circuits in these layers; and on the monolithic integration of such components with Si circuits fabricated on the same wafer. This effort is based on the significant potential that epitaxial growth of dissimilar semiconductor materials holds for technological applications. Nevertheless, relatively little theoretical work has been performed to understand the fundamental interactions and global issues governing the initial stages of growth and the structure of the first few mono-layers in these systems.

Of specific interest, for example, are the prototypical optically active systems GaAs on Si(100) and GaN on SiC/Si [6,7]. At present, optoelectronics involves growth of materials like GaAs (an optical material because of its direct band-gap) on substrates of Si (an electronic material with an indirect band-gap). For the future, GaN is of particular interest for optoelectronics applications in the blue and near UV because of its *direct* wide band gaps [5]. Unfortunately, the large lattice constant mismatches between the substrates and the epitaxial layers cause many defects to be created and propagate from the interface (see Table 1). Moreover, this is exacerbated by the interface charge mismatch caused by polarity differences between GaAs and Si. To resolve both problems, we invented a novel material specifically designed to consist of four-to-six types of atoms which *on the average* behave like Ga or As, by a systematic *ab-initio* exploration of the geometric, electronic and optical properties of a new class of compound semiconductors. The flexibility in the choice of ordering and sizes of atoms is used to (1) match the polarity of the substrate surface, (2) eliminate the

Table 1: Typical materials used in the electronics industry and their experimental lattice constant mismatch relative to Si $\Delta a/a_{Si}$ [8]. Most of the materials have a large lattice constant mismatch with Si. For those with a small lattice constant mismatch, there is still the problem of polarity mismatch.}

Compound	$\Delta a/a_{Si}$[%]	Polar
Si	0	no
Ge	+4.16	no
CuCl	-0.46	yes
ZnS	-0.41	yes
GaP	+0.37	yes
AlAs	+3.48	yes
GaAs	+4.11	yes
ZnSe	+4.36	yes
InP	+8.06	yes
InAs	+11.14	yes

lattice mismatch and (3) tune other properties, such as obtaining a direct band-gap.

In cases where two tetrahedrally coordinated compounds can not grow directly on top of each other because of large lattice mismatches and/or polarity mismatches, a set of these new materials of gradually changing lattice constants can serve as buffer layers to bridge between the two target materials.

The central piece to the new material is an epitaxial ordering scheme that ensures polarity matching between the new material and any substrates. The procedure starts with a tetrahedrally coordinated homopolar substrate, such as Si(100). A layer of group V elements is then deposited on top of it, followed by a layer of group II elements, then a layer of group V elements and finally a layer of group IV elements. This completes a cycle of elements in the growth direction, from group IV, to group V, to group II, to group V, and back to group IV. The procedure can then be repeated. The electrostatic potential in the growth direction has the same periodic structure. Thus, there is no long range field effect, in contrast to the case of growing III-V material on top of group IV substrate (see Figure 1). Hence, the charge mismatch problem of the interface is eliminated. Furthermore, there is much flexibility on the types of atoms one can use. In principle, each layer can be of a different element, as long as it belongs to the correct group, this gives the designer many choices in adjusting for other physical properties. This new material can be written in a short-hand chemical formula $(\text{II-IV})_{1/2}\text{V}$, while it is understood that there may be more than one component to any of the three groups. For example, given group II atoms Zn, Cd, group IV atoms Si, Ge, and group V atoms P, As, one could form compound ... Si P Zn As Ge As Cd As Si .... We will denote this class of material as Class I.

To achieve the same effect, we may also follow a different combination. We may start the deposition with a layer of group III element, followed by group

VI, group III, and then back to group IV. Written in chemical formula, this is $III(IV\text{-}VI)_{1/2}$, which we will call Class II.

Both Class I and Class II solve the polarity mismatch problem. It is clear that combinations of the two classes may also be considered.

substrate – Class I / Class II – Class I / Class II –...

Moreover, the procedure is not limited to homopolar group IV substrates. When some heteropolar substrate is used, such as GaAs, we can simply start the procedure from the appropriate layer. For example, the layering order can be

... III V III V IV V II V IV ...

or

... III V III V II V IV V II V IV ...

These procedures leave the material designers with many choices. Different types of atoms and different layering orders can all play a role in influencing the lattice constant and other properties of the resulting material. Since some materials will certainly be easier to fabricate than others, it is also important to accumulate a large pool of candidate materials for various lattice constants and other properties.

We are currently performing *ab-initio* total energy calculations, as well as *ab-initio* quasiparticle energy calculations, in order to discover the specific choices of atoms necessary to identify the optimal materials for heteroepitaxial growth on Si.

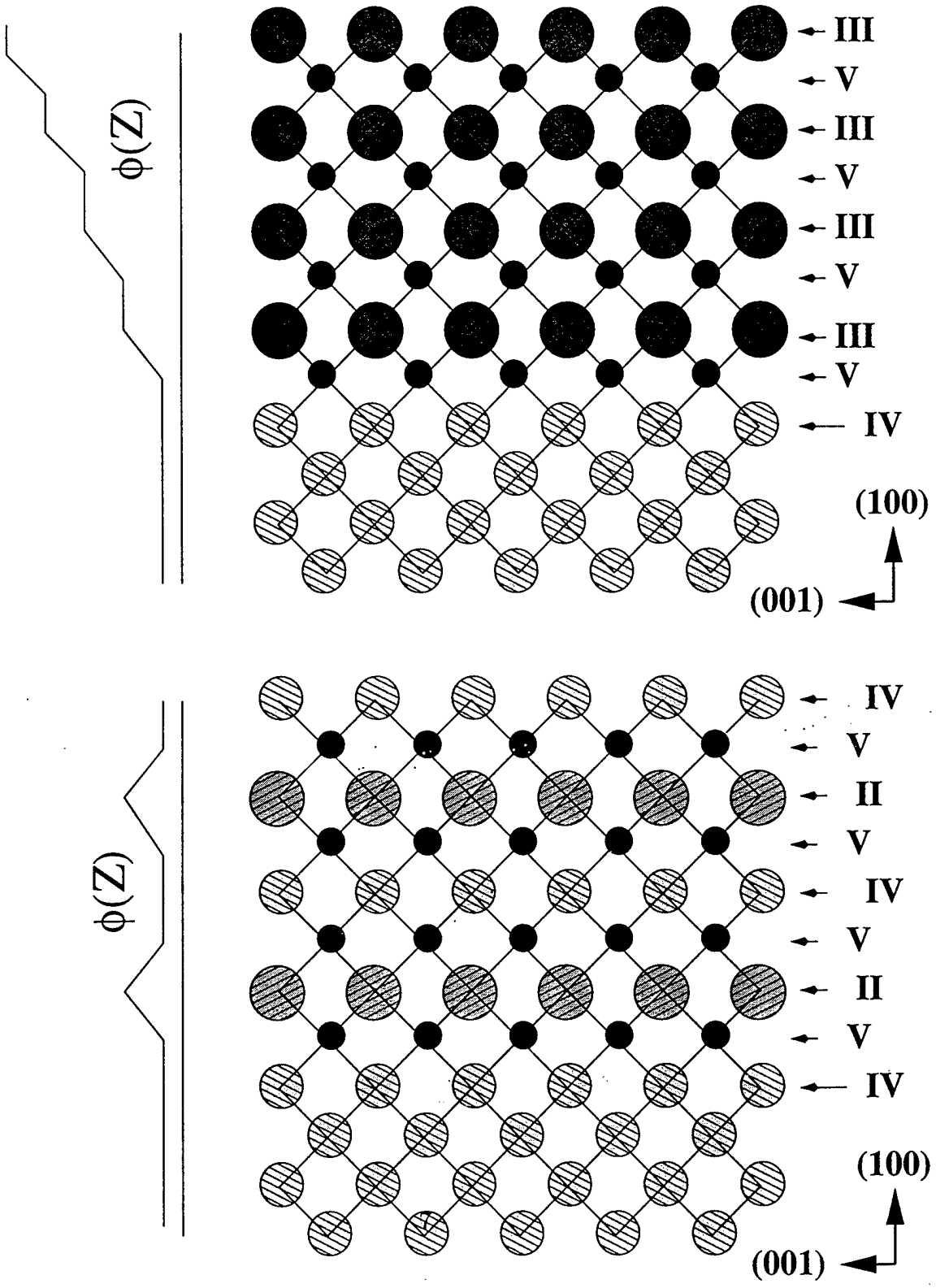

Figure 1: Illustration of epitaxial layering of Class I materials, compared with III-V materials. Note that the new material does not have long range field effect, in contrast to III-V materials.

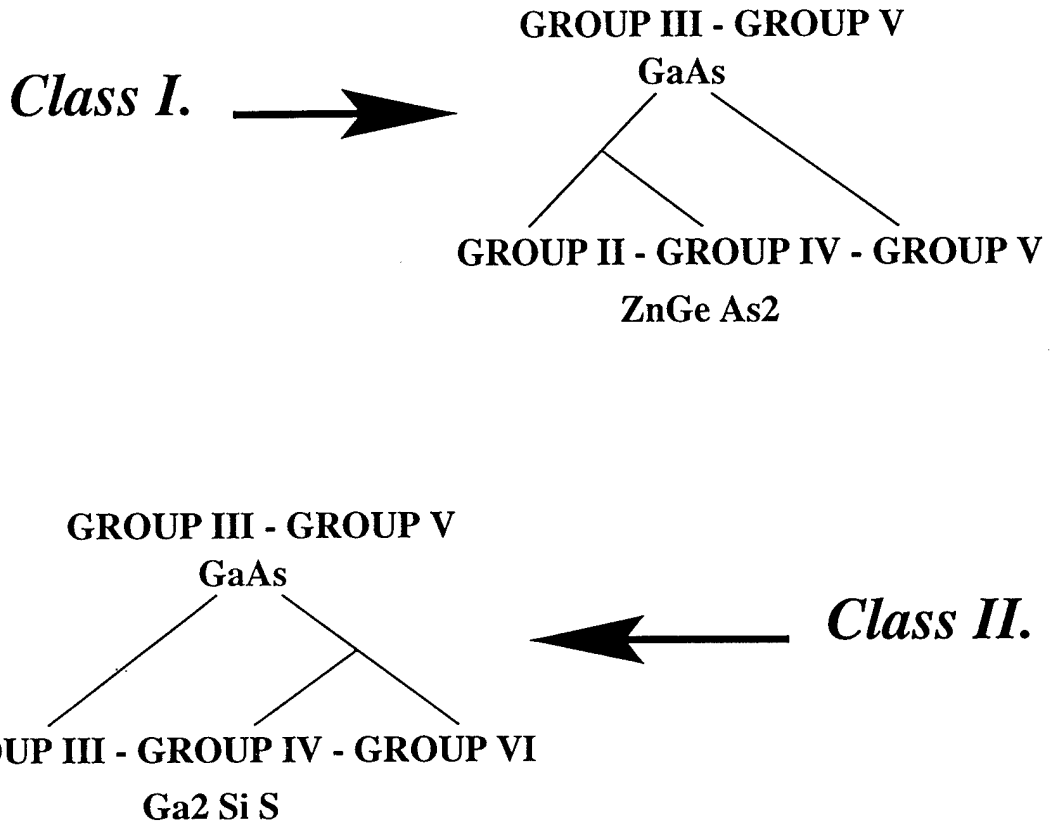

Figure 2: Class I materials are composed of group II, IV, V elements. One example is $ZnGeAs_2$. Class II materials are composed of group III, IV, VI elements. One example is Ga_2SiS.

References

1. *Heteroepitaxy in Silicon II*, ed. J. Fan, J. Phillips and B.-Y. Tsaur, MRS Symposia Proceedings N. 91 (Materials Research Society, Pittsburgh, PA, 1987).
2. R. F. Davis, *Proc. IEEE* **79**, 702 (1991).
3. J. H. Edgar, *J. Mater. Res.* **7**, 235 (1992).
4. C. R. Eddy, Jr., T. D. Moustakas and J. Scanlon, *J. Appl. Phys.* **73**, 448 (1993).
5. For a good review on GaN and other wide band-gap semiconductors, see J. E. Edgar, *M. Mater. Res.* **7**, 235 (1992).
6. T. Sasaki and T. Matsuoka, J. Appl. Phys. **64**, 4531 (1988).
7. Z. Sitar, L. L. Smith, and R. F. Davis, *J. Cryst. Growth* **141**, 11 (1994).
8. M. L. Cohen, Electronic structure and optical properties of semiconductors

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