Amorphous Silicon

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Abstract

The atomic arrangemnt is the case is not unique as in the crystalline materils, and enormours amount of structural disorder can take place. As the longe-range order of the atomic arrangement is completely lost a discussion based on reciprocal lattice space is meaningless. Amorphous Silicon has substantially different properties as compared to crystalline silicon. It has therefore become recognized as a fascinating and important material in its own right, with many interesting facets that lead to a range of novel and still developing applications. Investigation of structural properties and some exciting applications of amorphous silicon is discussed.

1 Introduction

In 1975, the silicon took the leading role, not only in the world of crystalline semiconductors, but also in the realm of amorphous semiconductors. At this stage, semiconductors meant crystalline semiconductors. Silicon technology was a general term for semiconductor technologies represented by large scale integration (LSI) based on crystalline silicon and had currently grown to a colossal entity, with LSI being regarded as rice of industry. Hence, those who had engaged in amorphous semiconductor research might well have been surprised with the predicted dominance of silicon in amorphous technologies. It should be noted, however, that amorphous silicon has substantially different properties as compared to crystalline silicon, and that research and development of amorphous silicon has taken place entirely different field, thus building up a technology of its own. This may be attributed to several factors. The science of amorphous semiconductors which deals with structural and electronic properties is far from complete, being still in a developing stage, and in place of the conventional solid state physics based on translational symmetry (long-range periodicity). The long-range order of the atomic arrangement is no longer existed here, therefore reciprocal lattice is meaningless.

A thin film of amorphous silicon contains a large amount of hydrogen,which plays an essential role in characteristics of such material. In fact, this new technology is dealing with a new material, different from conventional amorphous silicon. To be exact, this material should be designated as hydrogenated amorphous silicon (a-Si: H). Though not yet fully completed, considerable amount of information has been accumulated in the last two decades, covering the microscopic analysis of the preparative process, state of hydrogen inclusion, structures, defects and electronic properties. A new discipline of amorphous silicon physics has been created, injecting a breath of fresh air in to material science.

2 The Structural Properties

2.1 Atomic Arrangement

The structure of amorphous silicon is characterized as an irregular arrangement of atoms in contrast with crystalline solids whose structure has a periodic array of atoms, as seen in Fig.1.

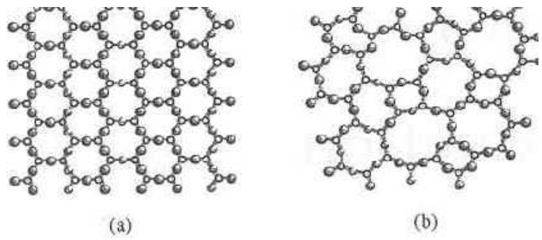

Figure 1: A hypothetical two dimentional oxide, A_2O_3: (a) Crystalline (b) Amorphous form [1].

Such a disordered structure manifests itself as a hollow pattern of electron as shown in Fig.2. This is contrast with that for crystalline silicon which exhibiting the Laue spots

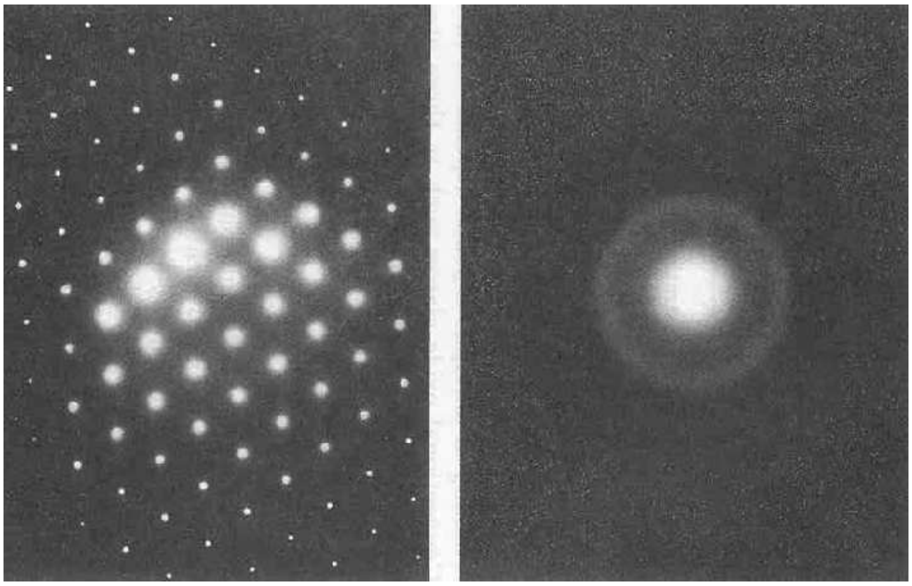

Figure 2: Electron diffraction patterns: (a) Crystalline silicon, (b) Amorphous silicon [1].

2.2 Diffraction pattern

From an amorphours material diffraction pattern, containing one or more broad diffuse rings, the only quantity which can be determined directly is the radial distribution fuction. This is obtained from a Fourier analysis of the experimantal x-ray scattering curve, and gives directly the average number of atoms to be found at any distance from a given atom. The method of Fourier analysis is equally applicable to a liquid, an amorphous or a powdered crystalline materiail [5]. It is convenient to begin the analysis of the diffraction pattern with the equation for the structrue factor of the basis.

$$S_{\mathbf{G}} = \sum_j f_j exp[-i\mathbf{G} \cdot \mathbf{r}_j]$$

Instead of writing it for the structure factor of the basis, we write the sum for all the atoms in the specimen. Further, instead of specializing the scattering to the reciprocal lattice vectors $\mathbf{G}$ characteristic of a crystal, we consider arbitary scattering vector $\Delta\mathbf{k} = \mathbf{k}' - \mathbf{k}$, we do this because scatering from amorphous materials is not limited to the reciprocal lattice vectors, which in any event cannot here be defined.

X-ray intensity $I(\mathbf{k})$ is expressed as a function of $\mathbf{k}$ for crystalline solid [1],

$$I(\mathbf{k}) = Nf^2\phi(\mathbf{k}) = Nf^2[1 + \frac{2}{N}\sum \frac{Sinkx_n}{kx_n}]$$

Where: f-atomic scattring factor, N- number of atoms and, $\phi(\mathbf{k})$ is the diffraction function.

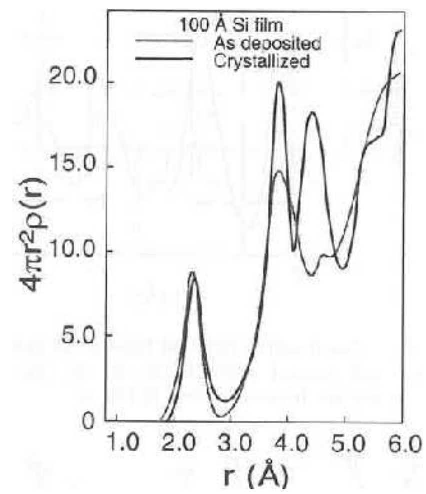

Figure 3: Radial distribution function of amorphous and crystalline Si as determined from analyses of electron diffraction data [1].

For liquid and amorphous materials, averaging on all orientations, $\phi(\mathbf{k})$ is given by,

$\phi(\mathbf{k}) = 1 + \int_0^\infty 4\pi r^2[\rho(r) - \rho_0]\frac{Sinkr}{kr}dr,$

Where $4\pi r^2\rho(r)$ is called radial distribution function and ρ_0 is the average density of atoms, So that $4\pi r^2\rho_0$ means radial distribution function for uniform distribution atoms.

$\rho(r)$ for a-Si are shown in Fig.3. The data were obtained from the Fourier transformation of the electron pattern for evaporated a-Si. Also $\rho(r)$ c-Si obtained from crystallization by thermal annealing of a-Si is shown for comparision [1].

3 Electronic properties

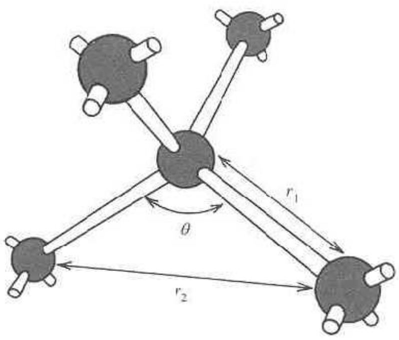

Figure 4: Illustration of short-range structural oredr based on sp^3 hybridized orbitals [2].

It is well known that the chemical-bond theory provides us with a simple physical understanding of electronic structure of crystalline semiconductors. This can also be applied to amorphous semiconductors [2].

Materials with hydrogen contents with ranging from ~ 1 to $\sim 60\%$ have been reported [4] that typically contain high concentrations of electronically active defects. Therefore, its room temperature conductivity could be made to vary in significant amount [3].

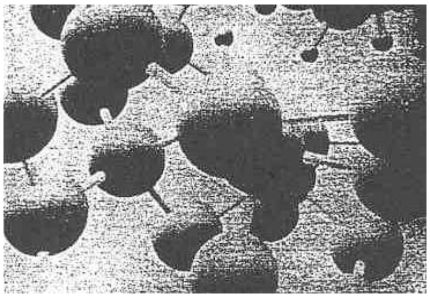

Figure 5: A model structure of a-Si:H. The big balls are Si, the small ones hydrogen atoms.

In amorphous hydrogenated silicon (a-Si:H) each atoms is bounded to the four other Si atoms surrounding it by four chemical bonds based on sp^3 hybrid orbitals, and locates itself at the center of gravity of a tetrahedron formed by the four neighbouring Si atoms. Here, eight hybride orbitals are separated into four bonding and four antibonding orbitals [2]. The bonding orbilats of lower energy are filled by four outer valence electrons supplied from each of the Si atoms, while the anti bonding orbitals remain empty. As a result of interaction between the adjecent orbitals, the bonding orbitals form a valence band filled with electrons, while antibonding orbitals form an empty conduction band, as schematically illustrated in Fig.6. A finite energy gap exist between the two bands, and as the Fermi level is located withing the gap, a-Si shows the properties of a semiconductor.

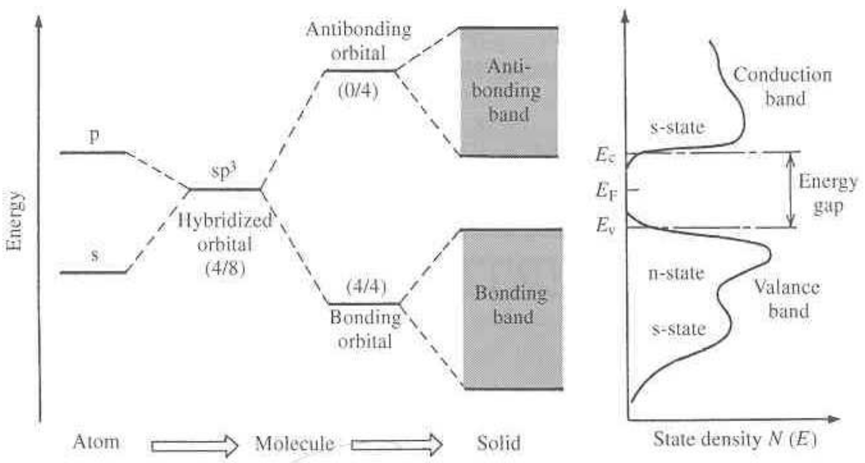

Figure 6: Band structure of tetrahedrally bonded semiconductor as portrayed by the use of chemical bond theory [2].

However in crystalline semiconductor with longe range-order, the wave vector **k** of the electron is a good quantum number for discribing the electronic state based on the Bloch theorem therefore dispersion relationship, between elecron energy E and the wave vector **k** is well defined. In the case of amorphous semiconductor the wave vector is no longer a good quantum number. In its place the energy density of state distribution function, $N(E)$ becomes the major subject [2] of the discussion of the electronic structure of a-Si.

4 Applications

Solar cell was the first commercial product containing amorphous Si, displaying low power consumption for calculator's liquid crystal display, operation under artificial illumination such as fluorescent lighting, and good matching with the spectral response of a-Si solar cells [2]. Since the optical absorption coefficient of a-Si is much larger than that of crystalline Si, film materials as thin as 1 micro are suitable; these can be prepared at low temperatures [3]. From the view of point resources, Si is one of most abundant elements on earth. These facts identify a-Si as the most promising candidate for use in solar cells in the future from the point of view of power generation. Other applications are Solid state photosensors such as color sensors, contact type linear image sensors, line sensors for X-ray computerized tomography. Also Field effect (thin-film) transistor [2] for Liquid Crystal Displys and Photoreceptor drums for electrophotography and laser-beam printers are also valuble examples.

References

[1] Physics of Amorphous Semiconductors, edited by Kazuo Morigaki (Hiroshima Institute of Technology, Japan).

[2] Amorphous Silocon, edited by Kazuhobu Tanaka, Elichi Maruyama, Toshikazu Shimada, Hiroaki Okamota, Translated by Takeshi Sato (National Institute for Advace Interdisciplinary Reaserch, Ibaraki, Japan).

[3] The Physics of Hydrogenated Amorphous Silicon I, edited by J D Joannopous and G. Lucovsky. (Struture, Preparation and Devices)Vol. 55.

[4] The Physics of Hydrogenated Amorphous Silicon II, edited by J D Joannopous and G. Lucovsky. (Electronic and Vibrational Properties) Vol. 56.

[5] Introduction to Solid State Physics, edited by Charles Kittel, Seventh Edition.