DEFECTS IN NON-CRYSTALLINE MATERIALS

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1. Introduction

Everybody knows what is a crystal, but what is a non-crystalline solid?

Many books describe the non-crystalline (amorphous and glassy) state of the solid as the state lacking the long-range ordering of the atoms. That means that a non-crystal is something, which is not a crystal.

The lack of a positive definition of the non-crystalline state of matter is due, after our opinion, to the fact that the non-crystalline structure cannot be specified by atomic co-ordinates but only by statistical parameters related to the assembly of the particles. It is somewhat similar to the case of the statistical mechanics applied to gases 150 years ago.

In order to study the defect states we must refer to some kind of ideal, non-crystalline state and then to discuss the deviation from this state as a state with defects embedded in it.

Some researchers define the ideal non-crystalline state as the state with the structure of the liquid stateof a given material but nobody knows what the real structure of a liquid is.

Other people suggest that an ideal glass should have a "relaxed" structure of assemblies of clusters with fivefold and icosahedral symmetry [1].

Stevels [2] tried to describe the ideal non-crystalline state by using the concept of repeatability number (*RN*). This number gives a measure of the degree of order of a network in a limited area defined by the radius r_0:

$$RN = \frac{3}{4\pi\, r_0^3} \int_0^{r_0} CRS\,(r) \cdot 4\pi\, r^2\, dr,$$

where *CRS (r)* is the coefficient of repetition in space and represents the average over the atoms situated in the area of the coefficient of the linear repetition CLR (the CLR is the number of atoms in the direction *x* in *n* steps divided by *n*). For a perfect crystal *RN*=1 and for the ideal amorphous solid *RN* should be zero.

While there are obvious divergences concerning the definition of the ideal non-crystalline state, physicists are unanimous in defining the disordered, amorphous, glassy, vitreous or generally non-crystalline state as a structure lacking *long-range order* (LRO) (i.e. atomic correlations up to very large distances) but retaining *short-range order* (i.e. atomic correlations in the first atomic shells).

The non-uniqueness of the amorphous state is the basis of various structure related modifications of properties in disordered materials: optical effects, photo-structural effects, radiation-induced effects, mechanical changes induced by thermal annealing without crystallization, etc.

How can we understand the differences between various forms of the same non-crystalline material, which exhibit different physical and chemical properties? We must deal with the concept of *defect in the disordered state*.

2. Defects in crystals

In crystalline solids the structural defects are defined in terms of the deviation from the ideal LRO of a given lattice. Three basic types of defects can be defined (Fig. 1):

     i) intrinsic point-defects (vacancies, interstitials)
     ii) chemical impurities (substitutional or interstitial atoms)
     iii) extended defects (dislocations, stacking faults, lattice distortions, colloids, grain boundaries)

It is worthwhile to mention a special kind of extended defect related to lattice distortions in a rather perfect crystal. If a binary crystal (AB crystal whom atoms, A and B, are characterized by significant difference between the atomic or ionic radii: e.g. A=Cd, B=Se) is grown such as to have, in one crystallographic direction, a decreasing concentration of one component, then one obtains a variable lattice parameter along the growth line. The crystal losses the translation periodicity in that direction. Such crystals are very important for applications. A special X-ray optics, based on such crystals, has been developed and procedures were patented [3].
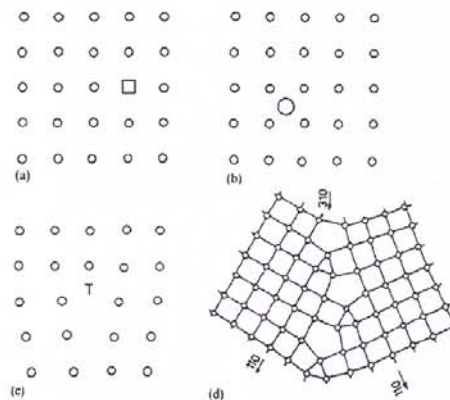

Fig.1 Defects in crystals: (a) vacancy; (b) interstitial; (c) dislocation; (d) grain boundary.

3. Are there well-defined defects in a non-crystalline solid?

The main problem to be discussed is: are there defects, which can be described as counterparts to the well-defined defects in crystals?

Although most defects seems to have lost their meaning and structure, the structurally sensitive changes in the properties of amorphous alloys show, at least qualitatively, the same trend as corresponding properties of crystals [4]. In crystals the changes of properties are governed by the behaviour of lattice defects. For example, annealing leads to the annihilation of dislocations and point defects whilst plastic deformation increases the density of both these lattice defects. The above observations allow concluding that structural defects, which are akin to defects in crystals, should exist in non-crystalline materials.

The deviation of the structure of a non-crystalline solid from its low energy equilibrium state could be, then, described in terms of the increase in the density of defects. Thus, structural relaxation is a process of annihilation of defects and is an exothermal process [5, 6]. In contrast, the mechanical deformation of a structurally relaxed alloy leads to the creation of defects, which is, naturally, an endothermic process.

In the light of the above considerations we cannot regard as a defect any small ordered domain formed in non-crystalline structures whereas in crystals small disordered regions are considered to be clusters of elementary defects.

Several attempts have been made to define the structural defects in non-crystalline solids on a general basis [7]. Firstly, an ideal reference structure is defined and the defects are introduced using geometrical concepts analogous to those used for crystal defects. The strains are measured with respects to the reference structure and they are always very high. However, this definition of defects, using the local strain seems to be valid only for covalently bonded solids [8].

Other descriptions focus their attention on one or two atoms only and fail to recognize the defects as collective phenomena [9]. Egami et al. [4] have defined the structural defects in amorphous alloys as sources of internal stresses and regions of a certain type of atomic site symmetry. In this approach, no ideal reference structure is needed and all the quantities are referred to the corresponding equilibrium, but not necessarily the lowest energy configuration of the atoms.

4. Defects in non-crystalline structures

Most defects are diffuse or collective defects. In this case, the deviation from the ideal network (if any) should be theoretically the best procedure for the characterization of such defects. We shall not discuss the diffuse defects in great detail. The other defects are local defects.

The local defects can be divided in:
a) intrinsic defects, which are characteristic to the material even after relaxation, and
b) extrinsic defects, which are annihilated during relaxation.

The local defects can be classified also as:
 i) point defects
 ii) extended defects
    - quasi-vacancy dislocation
    - quasi-interstitial dislocation
    - domain boundaries between two amorphous phases.

We add to these classification various kinds of chemical defects.
The macro-defects are defects at the scale of the supernetwork:
    i) voids
    ii) pinholes
    iii) cracks
    iv) network of pores

5. The characterisation of the defects in non-crystalline structures and their influence on the physical properties of the material

5.1. The point defects

Let's study the problem of the vacancy and interstitial in non-crystalline structures.

In the case of amorphous metal structures, where directional bonding is lacking, a vacancy defect is not stable. When a vacancy is produced into such structure then it rapidly collapses.

Spaepen [10] simulated the dynamic properties of a disordered system with 3000 spheres. He analysed the evolution of a vacancy created in the system by picking out a sphere at a given moment (Fig. 2). The free volume thus created was rapidly redistributed and the vacancy lost its identity as a localised point defect.
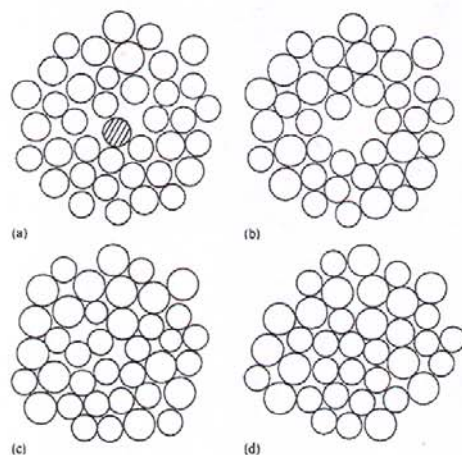
*Fig. 2 Sequence of configurations illustrating the collapse of a vacancy in the
two-dimensional dynamic hard sphere experiment: (a) initial structure; (b) after
the shaded atom has been picked out; (c) intermediate stage of simulation;
(d) final configuration illustrating the disappearance of the vacancy.*

The same type of simulation was carried out by Bennett et al. [11] on a three-dimensional
dense random packing model and got the same effect: the instability of a vacancy point defect. This is
in sharp contrast with the case of hard sphere dynamic simulation in crystalline arrays. Therefore, as
a consequence of long-range elastic strain fields, during the rearrangement at the vacancy site, the
displacements of the local collapse can be transferred to the specimen boundary. That is why we
cannot consider a vacancy-type point defect as a possible defect in amorphous structures based on
non-directional bonding of the atoms.

The same thing happens in the case of the interstitial atoms.

In covalently bonded solids, as e.g. tetrahedral semiconductors, the vacancy-like defects or
quasi-vacancy defects can occur as an usual defect and can be defined as a local arrangement of
atoms which implies lower density than the average density of the material. Although,
experimentally, it is not possible to observe such quasi-vacancies, the simulation of the disordered
network using modern modelling procedures allowed to characterize the structure of the
quasi-vacancies, their distribution, and dynamic properties.

In the ideal network the density distribution is uniform. In the real networks the bonding
fluctuations determine the density fluctuation and, therefore, the formation of quasi-vacancies and
quasi-interstitials can be obtained by simulating the local disorder in crystalline silicon (Ge).

It is interesting to remark that the best evidence and characterization of a couple of
quasi-vacancy - quasi-interstitial can be obtained by simulating the local disorder in crystalline
tetrahedrally bonded semiconductors. If, by a particular event, e.g. the impact of a very energetic
particle, a local defect is produced in silicon (germanium) lattice, then the lattice can restore its
bonding but in a different configuration. The restoring creates a local deformation. In fact, the
deformed state is characterized by the formation of four 5-fold rings of atoms and two 7-fold rings of
atoms that correspond to two strongly related regions with a lower and, respectively, higher local
density, i.e. a quasi vacancy-interstitial pair or quasi-Frenkel defect.

The distorted region encompasses ≈1 nm and contains a cluster of 26 atoms. The free energy
rise is moderate and therefore such defects have good stability. Although rare in crystalline
tetrahedrally bonded semiconductors, such quasi-Frenkel regions are formed as a rule in non-
crystalline semiconductors.

We have called this defect: *deformon state* or simply *deformon* [12].

In amorphous metallic materials high stress and low stress regions were revealed and these narrow regions can be associated with the quasi-vacancy or quasi-interstitial defects.

Egami et al. [4] defined the defects in amorphous alloys as source of internal stresses and regions of a certain type of atomic site symmetry. In this case, an ideal reference structure is needed. They applied the analysis of the defect structure to the computer-simulated model of amorphous metal (Fe) [13]. A cluster of 2067 atoms in a box was relaxed and the stresses in every atom position were calculated.

The first striking result of the analysis of the internal stresses is that, unlike any ideal crystalline structure, the amorphous structure exhibits high internal stresses (Fig. 3).
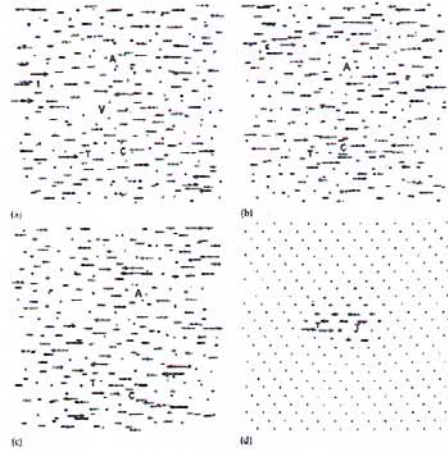

Fig. 3 The stresses in three successive layers (a, b and c) of a model of amorphous iron (a-Fe) and (d) in crystalline iron (d) for the block containing an edge dislocation.
A - low stress region; C - compressed region; T- tensile region

Stresses of similar magnitude exist in the cores of crystalline dislocation. The environments of individual atoms differ significantly from one atom to another. Although the distribution of stresses is random over the whole model, appreciable correlations exist locally among the neighbouring atoms, so that it is possible to identify regions containing 10-20 atoms with either low internal stresses or high symmetry and high internal stresses and low symmetry. Tensile and compressive regions are neighbouring. It is quite remarkable the strong resemblance of the stress distributions in an amorphous material, and a crystal if one judge after figure 3d where the distribution of the hydrostatic stress for an edge dislocation in the crystalline lattice is shown.

In conclusion, what is point defect in crystalline lattice is a narrow region defect in a non-crystalline network.

An other type of defect proved to exist and to play a leading role in the non-crystalline semiconductors is the so-called dangling bond (d.b.). A single dangling bond defect, i.e. an unsatisfied bond (Fig. 4) can be incorporated within the network without much perturbance of the surroundings; on the contrary, it helps to reduce the strains accumulated during network construction.

Fig. 4 A dangling bond in a continuously interconnected tetrahedrally bonded random network (Si, Ge).

The dangling bond was ascribed to the dominant paramagnetic centre in non-crystalline films based on amorphous silicon (a-Si) and hydrogenated a-Si (a-Si:H). The centre exhibits a g-value of 2.0055. The close correlation between the photoluminescence efficiency and the spin density in a-Si:H indicates that the distribution of the paramagnetic defect centres is nearly random [14].

Until 1986, it was almost universally believed that a single point defect, namely the dangling bond, dominated the properties of a-Si.

Pantelides [15] has brought arguments in favour of the existence of both threefold and fivefold co-ordinated atoms as defect centres. One argument is that in amorphous silicon a vacancy, which introduces a threefold co-ordinated system and a tetrahedral self-interstitial, (which introduces 4 fivefold co-ordinated silicon atoms) has roughly the same formation energy. A number of examples of that nature seem to prefer five-fold over three-fold Si were also given. An other argument is the recent development of techniques for the routine synthesis of chemical compounds involving five-fold co-ordinated silicon atoms (called pentacoordinate silicon) [16].

Pantelides defined the counterpart of dangling bond for five-fold co-ordinated silicon as *floating bond* (f.b.). Ideal dangling bonds and floating bonds are rarely produced. In general an intermediary state is produced and this configuration was called *frustrated bond*. Pantelides proposed that the defect centre is likely to be mobile because of the ease to switch bonds. The enhanced H-diffusion caused by doping [17] and by illumination [18] are explained in a unified and simple manner in terms of excess defect centres which are mobile and kick out H atoms from Si-H bonds [19].

One particular and very important defect was firmly established in chalcogenide glasses. These glasses are based on the chalcogens: sulphur, selenium and tellurium and combinations thereof, including alloys with various covalent elements.

Kastner et al. [20] proposed ~20 years ago that the energetically least-costly bonding deviations in chalcogenide materials can be achieved when two defects are always created at the same time: a positively charged overcoordinated atom and a negatively charged undercoordinated atom. These are called valence-alternation pairs (VAP) because the valence or co-ordination is alternated for the defect atoms.

Fig. 5 shows how in amorphous selenium matrix two selenium atoms, each of which is triply bonded, serve to cross-link two molecular chains of double bonded atoms. A VAP can be produced by a spontaneous breaking of the cross-linkage, combined with the simultaneous transfer of an electron from one of the triply bonded selenium atoms to an atom near that where the cross-link was broken. Since such electronic transfers reduce the total energy of the solid, nearly all the trigonally bonded selenium atoms become members of such valence alternation pairs.
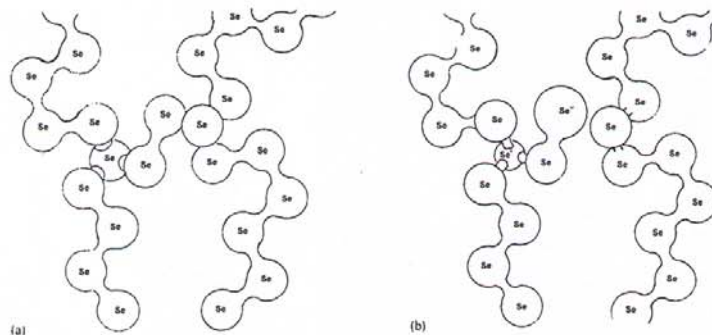

Fig. 5 *Valence alternation pairs in amorphous selenium (a-Se): (a) two selenium atoms cross-link two molecular chains; (b) a valence alternation pair is produced by spontaneous breaking of the cross-linkage.*

Since the total number of bonds in the solid does not change by creating these defects two at a time, the energy needed for creation of a pair is relatively small. It is approximately the energy required to place the negative charge onto the undercoordinated atom (reduced by relaxation effects of the surrounding matrix). In typical chalcogenide glasses this results in a VAP defect density of

about 10^{17} cm^{-3}, in agreement with defect densities measured by photo-induced spin resonance and absorption and by photoluminescence [21].

The VAP defect centres are normally diamagnetic. Exposure of chalcogenides to light at low temperatures brings these centres, by capture of photo-excited charge-carriers, into their neutral and paramagnetic state [21]. The VAP centres can also be photo-created because the energy required is less than the optical gap energy. These VAP centres have all the features of the defects postulated earlier by Street and Mott [22] for explaining a large number of electronic properties of chalcogenide glasses. In particular, these defects are associated with a negative effective correlation energy, which means that the reaction

$$2D_0 \rightarrow D^+ + D^-$$
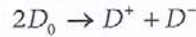
is exothermal and that the charged defect centres can interconvert by charge transfer into their oppositely changed counterpart:

$$e + D^- \leftrightarrow D^0 \leftrightarrow D^- + h$$
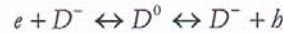
Here D^0, D^+ and D^- denote the different charge states of a defect centre. In the VAP model the defects can be a group V, VI or VIII atom; group IV atoms are ruled out because their co-ordination cannot exceed four in a covalent matrix. Hence, bounding constraints may hinder the interconversion expressed by the above relaxation for some defects in solids containing appreciable amounts of group IV atoms [23]. Photo-luminescence data are of leading importance in the development of defect models.

A more general defect in chalcogenide glasses, the quasi-molecular defect (QMD), was proposed by Popov [24].

The quasi-molecular defect is a single orbital-deficient bond against the covalent background. The formation of the simplest QMD in selenium is shown in Fig. 6.
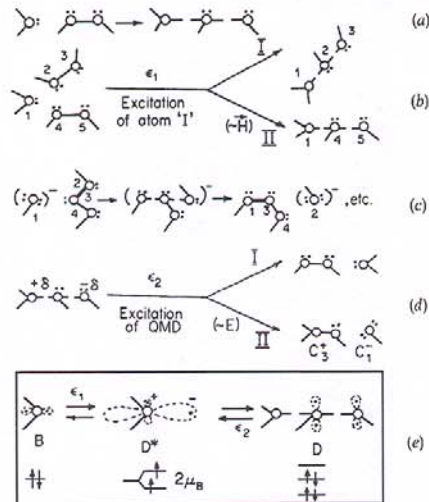

Fig. 6 Quasi-molecular defect and elementary processes that involve QMDs (after [25])
(a, b) QMD formation; (c) covalent bond switching; (d) QMD destruction;
(e) model for the excited state D*.
O - the selenium atom: - lone-pair p-electrons; —— covalent bonds;
---- orbital deficient bonds. The dotted drawing is a p-orbital.

In contrast to a covalent bond, which is established by electron pairing between two atoms, an orbital-deficient bond is a multi-centered one, so a QMD is a multi-atomic (or molecular) defect. From the properties of orbital-deficient bonds, it follows that the three atoms in QMD under

consideration are bound more weakly than in the covalent case and are arranged along a straight line with definite length.

QMD is regarded as the characteristic defect in glass-forming substances [25]. QMDs play the dominant role because they take part in all processes, including VAP formation.

QMDs can explain the photostructural transformations in chalcogenide glasses, the basical phenomena for applications in optoelectronics. The photostructural modifications are proper only to the non-crystalline state of chalcogenides and can be attributed to the region of frozen defects in a conservative structure, i.e. in a network where the bond-switching between atoms is absent. Small structural changes with some distortion are caused by the movement of frozen defects through a structure, with this movement being excited by the strongly absorbed light [26].

5.2 Extended defects

The extended defects in amorphous covalent solids are still controversial. Disjunctions, disclinations or dislocation lines with variable Burgers vectors are discussed in the literature.

The disclinations are defined in elastic bodies as line defects similar to dislocations but differing in that rotations rather than translations constitute the operations involved. Gilman [27] used this concept to explain the flow properties of the non-crystalline, glassy materials.

In Fig. 7 two dislocations lines are compared in crystalline and vitreous silica. In the crystalline case there is a constant Burgers' vector along the line and the structure left behind as the dislocation moves is the perfectly restored crystal. In the non-crystalline case, the local translations that are needed to restore the bonding vary along the line length, so that the Burgers vector fluctuates in magnitude and direction.
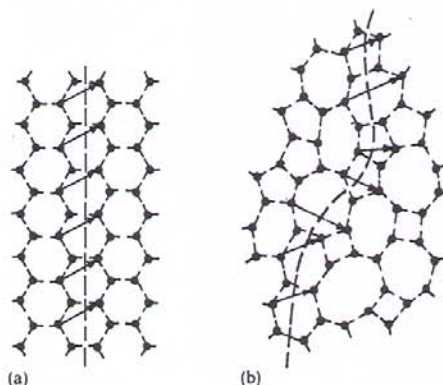

(a)   (b)

Fig. 7 Dislocation line in crystalline SiO$_2$ (a) and disclination line in vitreous silica (b).
The arrows indicate the Burgers vectors.

Rivier [28] has shown that odd-membered rings in a continuous random network (CRN) constitute line defects and that the disclination line may be described as threading its way through the glass by connecting the centres of the odd-member rings.

The theory of the defects in ordered media was extended to disordered solids in order to show that the existence of line defects associated with rotations (disclinations) is consistent with the absence of rotational symmetry in the material.

It is a paradox that, in spite of the theory, a very distorted structure, e.g. the model of germanium amorphous semiconductor, with only even-member rings of atoms, devised by Connell and Temkin [29], does not contain extended line defects.

On the other hand, in models of amorphous metallic alloys can be observed disclination lines, clearly resolved. In the dense random packing (DRP) model devised by Bernal [30] there were evidenced atomic collineations, a kind of disclination lines.

The disclination lines tend to approach the dislocation characteristics. The disclinations can be regarded as defective dislocations.

An alternative approach is to use the concepts of quasi-vacancy and quasi-interstitial [31]. The source of the formation of defect structures in non-crystalline alloys is the free volumes due to the high expansion coefficients in the liquid state. During the rapid quenching process, the liquid structure is undercooled, thus conserving partially the free volumes of the liquid state. Because of the difference in the atomic radii of the ions, at least in binary alloys, an optimum densely packed lattice cannot be formed, leading to empty spaces between the atoms. It is suggested that just below the glass transition temperature, T_g, these empty states are rather mobile. These are quasi-vacancies. Free volumes can agglomerate and migrate towards the surface and only small volumes may be stable as holes. In the same time regions of dense packing can appear. These are the quasi-interstitials. In the next stage the structure relaxes to a more stable state and this relaxation induces stresses which corresponds to the formation of so-called quasi-dislocation dipoles as discussed by Grimm and Krönmüller [32] (Fig. 8).
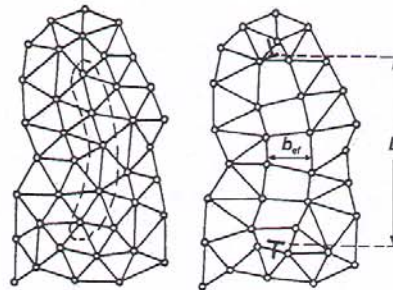

Fig. 8 Two-dimensional model of a quasi-dislocation dipole in an amorphous structure. The extraction of a "lattice plane" by a free volume accumulation and the subsequent relaxation is shown. b_{eff} is the effective Burgers vector and D is the dipole width.

Spaepen [10] has demonstrated that when a true dislocation is created in a disordered model, it becomes rapidly diffuse and loses its identity.

One of the most recent developments in the field of extended defects is the demonstration of the existence of boundaries between rather ideal non-crystalline regions. The ideal amorphous domain, the amorphite, is naturally introduced, because it was demonstrated by simulation experiments that the total distortion energy (free energy) diminishes by the fragmentation of the homogeneous random network into domains with nanometric size (Fig. 9). The interconnected amorphites exhibit distorted bonds at the boundary but not, necessarily, dangling bonds. The boundaries between amorphites are responsible for the specific properties of a-Si:H, especially for the reduced gap states of this material [33].
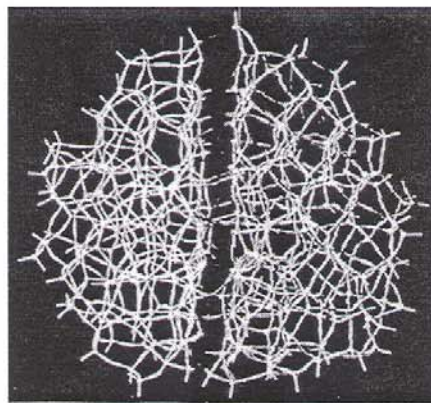

Fig. 9 The structural model for amorphous silicon (405 atoms) with two non-crystalline domains (amorphites).

5.3 Chemical defects

The most representative chemical defect is the wrong bond. For non-crystalline alloys of two or more elements the deviation of the structure from the ideal non-crystalline network is mainly dictated by the wrong position of some atoms in the network sites. Thus, in binary covalently bonded amorphous alloys (e.g. GaAs) the structure of minimum free energy corresponds to a network of bonds where every arsenic atom is bonded by gallium atoms and every gallium atom is bonded by arsenic atoms. The Ga-As bond is, energetically, the most favourable bond. Nevertheless, defects can be produced as bonds between atoms of the same type. These are the so-called wrong bonds (w.b.) and they play a leading role in controlling the properties of disordered compound semiconductors (Fig. 10).
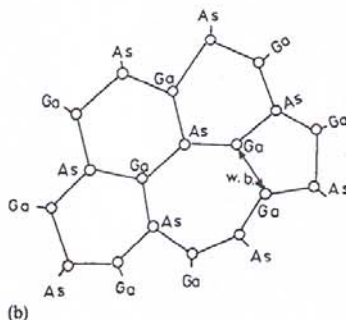

Fig. 10 Wrong bond (w.b.) in the non-crystalline network of GaAs.

In the classical models of amorphous semiconductors (Ge, Si) the six-fold rings of atoms, which are the basical configuration in crystals, alternate with five and seven-fold rings. In such case, the models applied to binary alloys include necessarily wrong bonds. Although these wrong bond defects cannot be avoided, their amount will be minimized, as demonstrated by the simulation of the structure of e.g. $CdGeAs_2$ glass [34] and comparison with experimental structural data.

The chemical additives can be incorporated into the basical network of the disordered semiconductors. As a rule, the non-crystalline semiconductors are difficult to be doped in the sense of the crystalline ones, because of the large number of the states situated in the forbidden gap and because of the possible accommodation of the impurity atoms, determined by the network flexibility.

In 1975, W.E. Spear demonstrated that the introduction of hydrogen atoms in small amount into amorphous silicon allows getting a dopable material. The gap states are greatly annihilated by hydrogen. The probable cause of this annihilation is the possibility of the VII-th group atoms (H, Cl, F...) to satisfy the d.b. bonds, thus eliminating the deep states associated with them.

In 1977 Ovshinsky and co-workers [35] discovered a way of incorporating certain additives into chalcogenide films, which increases their electrical conduction by many orders of magnitude.

Extrinsic conduction was achieved by "chemical modifying" the non-crystalline semiconductors with nickel or other transition metals. Highly doped $Ge_{32}Te_{32}Se_{32}As_4$ were n-type semiconductor.

There was possible to change the equilibrium concentration between the positively and negatively charged d.b. by incorporation of Ni, Fe, Cu, Cd. The incorporation of alkali metals as lithium and also of Bi and Sn metals, produced n-type conduction. In this case, pairs of their electrons should be given up to the positively charged d.b., converting them to negatively charged d.b.

5.4 Macro-defects

Of course, defects at a larger scale, the macro-defects, as e.g. voids, pinholes, cracks, porous structures, especially in thin solid films, are important features of the non-crystalline materials. Careful preparation can minimize these defects but the interaction between the micro and macro-defects deserves much investigation in the future. In some cases, as e.g. the porous structure, the large defect development is the goal of the producers.

We shall discuss here only the case of porous structure, because the discovery of porous silicon photo and electro-luminescence is the greatest discovery in the material science at the end of this century.

In 1990, Canham [36] discovered that, by a simple electrochemical procedure, it is possible to make at the surface of a silicon wafer an intricate network of channels which gives rise to nanodimensional structures able to exhibit intense photoluminescence (PL) properties (Fig. 11).
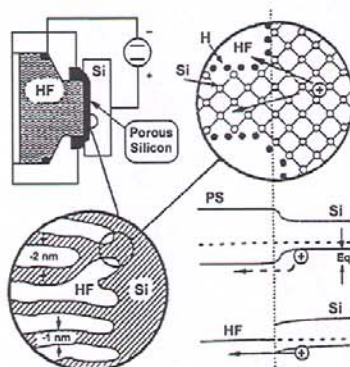

Fig. 11 Schematic diagram of a porous silicon electrochemical cell, porous silicon morphology and electronic junction structure used to explain the mechanism of the naturally self-limiting process for nanometer structure formation.

Detailed studies performed last years succeeded to show more and more convincingly that the PL effect is related to quantum confinement in small size silicon lattice.

The PL effect is strikingly different in crystalline porous silicon and in amorphous porous silicon. The macro-defects in both cases delimitate the nanometric size material parts with quantum confinement properties. The quantum energy levels of electrons in a potential well of dimension D vary like $1/D^2$. The decrease of the mean size of the silicon columns in the porous structure when the etching process is advanced, increases the energies of transition, resulting in a large blue shift of PL, as observed.

In a-Si:H the situation is quite different. Because of the disordered nature of the material, the wave function is strongly localized, in a range, which is much smaller than the nanosize structure. The spatial confinement responsible for intense PL does not produce any quantum effect and no blue shift is therefore observed when the size of the silicon entities are diminished by etching [37].

The porous silicon case demonstrates how the macro-defects in the disordered structure can control in a more or less direct way the quantum properties of the material and this fact challenges the development of the future applications of non-crystalline materials in optoelectronics.

6. Conclusions

The problem of the defects in disordered materials is one of the most challenging problems for the solid state physics. While the defects in crystals are known in details and their relation with the material properties is now enough well understood, in non-crystalline solids, the defect formation, classification and influence on the various physical properties of the disordered material are still open questions.

Nevertheless, experimental and modelling studies allowed for some preliminary conclusions.

Firstly, it is possible to identify particular defects that are counterpart of the crystal defects, although with obvious differences.

Secondly, the point defects and the extended defects in disordered solids are more diffuse as compared to those from the parented crystals.

Thirdly, new type of defects are possible, e.g. valence alternation pairs and quasi-molecular defects, which can be largely used for the control of the opto-electronical properties of relevance in applications.

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