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A NEW MODEL FOR THE DIFFUSION BEHAVIOR OF HYDROGEN IN METALLIC GLASSES

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Abstract—Both experimental and simulation results have indicated the deviation from Arrhenius law of the diffusion coefficient of hydrogen in metallic glasses. This deviation was traditionally explained by the existence of various kinds of jumps or in terms of continuous distributions of activation energies due to different kinds of disorder. A new model is suggested, which relates this deviation to the temperature dependence of the short-range order (SRO). The suggested model is applied to simulate the diffusion behavior of hydrogen in dilute amorphous Fe–H, Fe–Si–H and Fe–B–H alloys. The effect of the alloying elements on the activation energy of hydrogen diffusion in amorphous iron is discussed in terms of their electronic structure and mean volume. *© 1999 Acta Metallurgica Inc. Published by Elsevier Science Ltd. All rights reserved.*

Keywords: Metallic glasses; Hydrogen; Diffusion; Iron

1. INTRODUCTION

The interaction of hydrogen with amorphous metals and alloys has been studied extensively during the last two decades (e.g. Refs [1–23]). These studies were motivated by either scientific or technological interest. Hydrogen in amorphous metals may be used as a probe to study the structure of the amorphous state. In addition, the study of hydrogen transport processes in the amorphous structure may enable a better understanding of the diffusion of hydrogen through grain boundaries and its interaction with structural defects (trapping) in crystalline metals. Various actual and potential applications of amorphous metals are concerned with exposure to hydrogen (e.g. improving the production and electrical properties of amorphous semiconductor structures, hydrogen storage technology, devices for fusion reactors, etc.). Therefore, the study of hydrogen embrittlement, hydrogen diffusion, characteristics of hydrogen absorption and desorption and hydrogen effects on the electrical and magnetic properties is of great importance.

Many structural models [1–9] have been suggested in order to explain hydrogen diffusion and absorption in amorphous alloys. Kirchheim and co-workers suggested [1–4] that hydrogen atoms might occupy a wide variety of interstitial sites, resulting from both chemical and geometrical configurations in the amorphous structure. Hence, a broad continuous distribution of interstitial site energies is used to explain the concentration dependence of the chemical potential of hydrogen and its diffusivity in amorphous metals. Due to theoretical considerations [10], the shape of this energy distribution can be related to the shape of the first peak of the radial distribution function (*RDF*), which is usually assumed to be of a Gaussian form for amorphous metals.

The idea that hydrogen might occupy interstitial sites in amorphous alloys, which are similar to the octahedral and tetrahedral interstitial sites in crystalline alloys, was suggested in various papers (see, e.g. Refs [3, 11]). This idea is based on measurements of similar values of hydrogen solubility [11], frequency factor (D_0) and activation energy of diffusion [3] in amorphous and in f.c.c. structures.

Techniques that can monitor motion over wide temperature ranges (above 100 deg) often exhibit anomalous temperature dependencies of the diffusion coefficient of hydrogen in metallic glasses, which simple Arrhenius models cannot describe [19]. Nuclear magnetic resonance (NMR) measurements, for example, have revealed non-Arrhenius character for amorphous $TiCuH_{1.41}$ and Zr_2PdH_x hydrides [19–22].

Numerous theoretical concepts and computer modeling, mainly based on Monte-Carlo simulations, have been used to forecast the diffusion of hydrogen in amorphous metals. Ahmadzadeh and Cantor [12] were probably the first ones to use the concept of varying site and saddle-point energies for diffusion of light interstitial atoms and to run Monte-Carlo calculations for amorphous metals. Kirchheim and Stolz [13] used similar simulations

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to study the effect of the presence/absence of distributions of site and saddle-point energies on the characteristics of hydrogen diffusion in amorphous metals. Assuming no distribution of site energies, either with or without distribution of saddle-point energies, the linear behavior of Arrhenius plots for the diffusion coefficient was obtained. Allowing for a distribution of site energies, however, resulted in a pronounced negative curvature. Belyakova *et al.* [14] combined computer modeling (Molecular Dynamics) and experiments in order to study the effect of hydrogen on the structural and thermodynamic properties of iron and its alloys in amorphous, liquid and solid states. Whereas hydrogen did not affect the SRO in the liquid state, it substantially increased the interatomic distances in the amorphous and crystalline states.

Two alternative concepts have been suggested to explain the deviation from Arrhenius law of hydrogen diffusivity in metallic glasses. According to the first concept, different activation energies correspond to a like number of local environments and jump processes. Discrete activation energies may arise from combinations of various kinds of allowed interstitial sites (e.g. those with tetrahedral or octahedral symmetry), various kinds of jumps (e.g. relatively rapid ones within localized regions as well as long-distance motion) or trapping of hydrogen atoms at various structural defects. Examples of this descriptive scheme are presented in Refs [19, 23]. According to the second concept, the local environments for interstitial hydrogen atoms may vary in a quasi-continuous manner due to the disorder in the metallic glass. These variations should affect the energies of a hydrogen atom both in the interstitial and saddle-point positions for classical hopping processes. This perception is the basis for all works that assume a Gaussian distribution of site energies (e.g. Refs [13, 24]).

These two approaches, however, should be treated with caution. On the one hand, any outlook of temperature-dependent discrete activation energies [20, 21] does not fit the results obtained using models of distribution functions [25]. On the other hand, many inconsistencies of the Gaussian distribution models arise from NMR, perturbed angular correlation (PAC) and quasi-elastic neutron scattering (QNS) experiments, as well as from Monte-Carlo simulations [19, 22].

The aim of our paper is twofold. The main objective is to describe a new model, which explains the deviation from Arrhenius law of hydrogen diffusivity in metallic glasses in terms of the SRO of the structure and its temperature dependence. In addition, we present the model which allows the influence of alloying elements on the activation energy of hydrogen diffusion in amorphous metals to be accounted for. This model is based mainly on the coherent potential approximation (CPA) widely used in modern quantum mechanics calculations of thermodynamic properties of partially ordered or disordered alloys [26–29]. To illustrate the applicability of our model, the results on hydrogen diffusion in dilute amorphous Fe–H, Fe–Si–H and Fe–B–H are presented. The selection of these chemical compositions was motivated by: (a) our current experimental work on hydrogen interaction with amorphous Fe–Si–B alloys; (b) the comprehensive data existing in the literature on the local structure of iron in its solid, amorphous and liquid states (e.g. Refs [30–34]); and (c) the comprehensive data existing on hydrogen diffusion in crystalline iron and in amorphous Fe-based alloys (e.g. Refs [15–18]).

2. MODELING PROCEDURE

2.1. Definition of the short-range order

Experimental measurements of the *RDF* are often used to characterize the local atomic arrangement in materials, including amorphous metals and alloys. Amorphous metals may be assumed as "frozen" liquids, with a *RDF* similar to that of liquid metals, though showing a characteristic splitting of the second peak [30].

Making use of the experimental *RDF* of an amorphous metal and its temperature dependence, one can calculate the coordination number as a function of temperature. However, since such information on amorphous iron was not available to us, we referred to the similarity between the first peak of the *RDF* of amorphous and liquid metals and used the experimental density function of liquid iron at $T = 1620°C$ from Ref. [33]. The Boltzmann-type distribution function was used to model the temperature behavior of the density function:

$$g(r) = \exp[-\phi(r)/k_B T] \tag{1}$$

where $g(r)$ is the density function, $\phi(r)$ the potential of the mean force [35], k_B the Boltzmann constant and T the absolute temperature.

Equation (1) may be treated also as the main contribution to the Percus–Yevick [36] or Born–Green [37] equations, which define the fine structure of liquid metals. This approximation also presents the main features of $g(r)$ in metallic systems: it yields reasonable values of the height of the first peak of $g(r)$ and qualitatively reflects the oscillations of $g(r)$ in the vicinity of $g(r) = 1$. These oscillations are related to the oscillating character of the interatomic interaction potential in metals. From the experimental data for $g(r)$ at a fixed temperature we can extract $\phi(r)$ and use it to model $g(r)$ at different temperatures. This procedure results in the density functions of liquid iron that are presented in Fig. 1.

The radial distribution function of the monoatomic amorphous solid can now be expressed by the following equation:

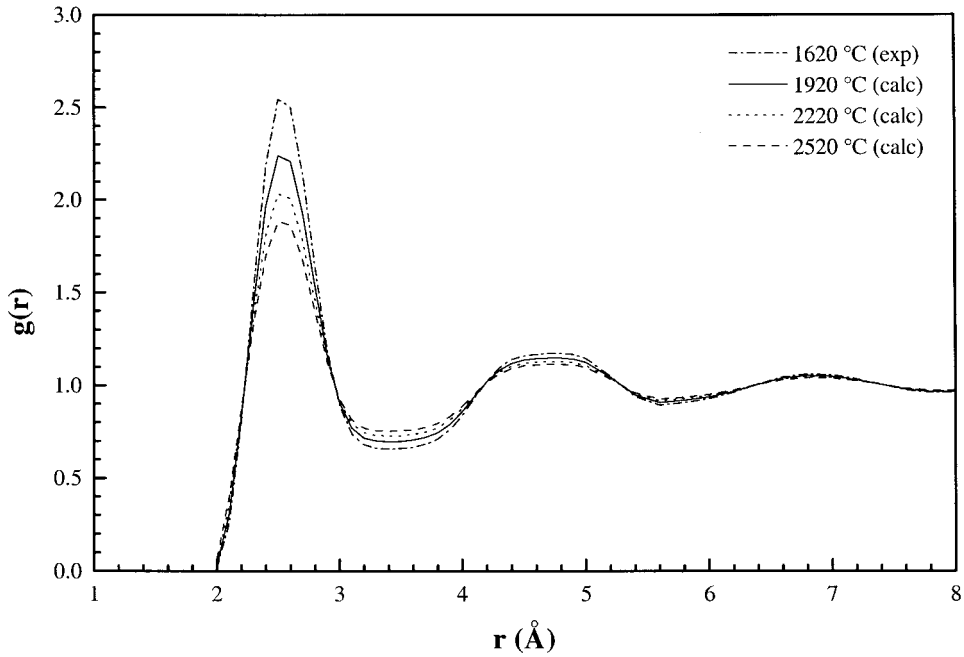

Fig. 1. The dependence of the density function of liquid iron on temperature, as calculated using an experimental density function and equation (1).

$$RDF(r) = 4\pi r^2 \rho(r) \tag{2}$$

where $\rho(r) = g(r)/\Omega$ is the local atomic density and Ω the mean volume per atom. We neglect the small changes in the value of Ω at varying temperatures and use the value of 13.44 Å^3 (90.79 a.u.^{3}) [33]. This way we can draw the *RDF* at different temperatures, as shown in Fig. 2 for $T = 1620°C$.

The coordination number (*CN*) can now be calculated by the routine integration procedure:

$$CN = 4\pi\rho_0 \int_{r_1}^{r_2} g(r) r^2 \, dr \tag{3}$$

where r_1 and r_2 are the limits of the relevant peak of the *RDF* and $\rho_0 = 1/\Omega$ is the mean atomic density.

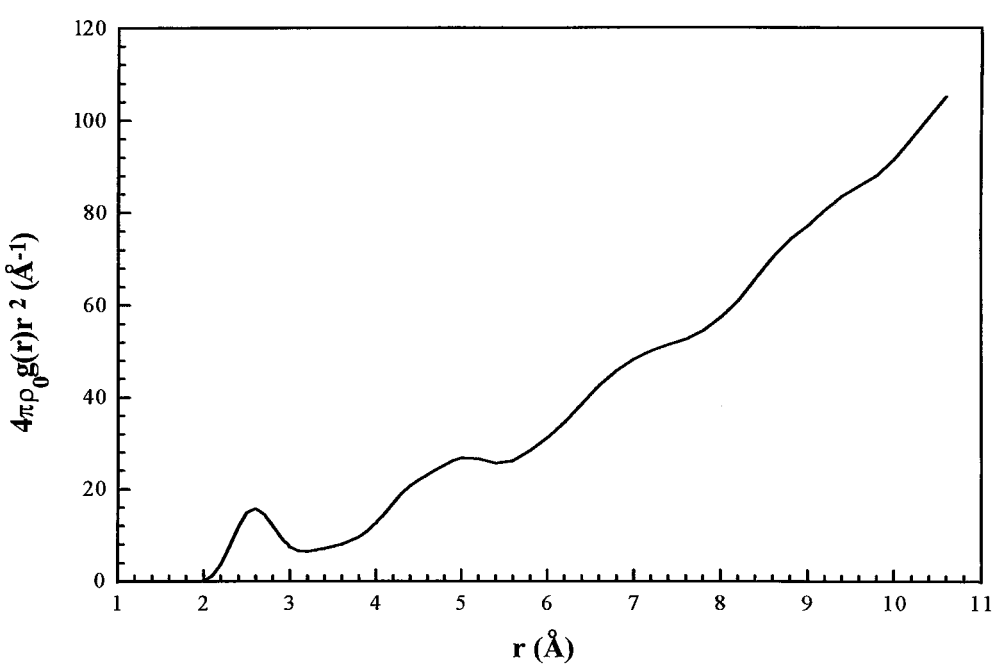

Fig. 2. The radial distribution function (*RDF*) of liquid iron at $T = 1620°C$, as calculated from equation (2).

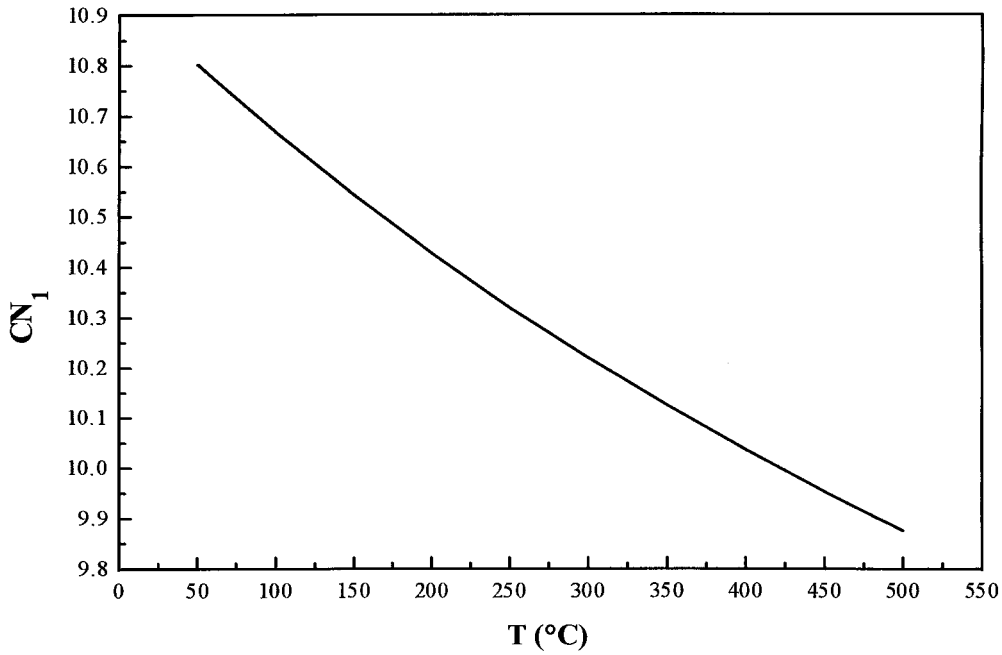

Fig. 3. The dependence of the first-shell coordination number of amorphous iron on temperature, calculated from equation (3) [38].

In order to calculate the first-shell coordination number (CN_1), one can either integrate directly the first peak of the *RDF* or run a Gaussian fitting of $g(r)$, then set it into equation (3). Using the first option and $g(r)$ at different temperatures, the temperature dependence of the first-shell coordination number that is displayed in Fig. 3 is obtained. In order to deal with an amorphous solid, all calculations were performed in the temperature range 50–500°C.

The observed decrease of the coordination number with temperature can be explained by substantial decrease and small broadening of the intensity of the density function at increased temperatures. It should be mentioned that the values of coordination number presented herein are in accordance with the experimental results of Ruppersberg and Seemann [34], who used X-ray testing of liquid iron to estimate the first-shell coordination number.

The second peak of the *RDF* of iron is not well defined (Fig. 2). However, on the basis of experimental measurements it was concluded [34] that liquid iron has a f.c.c. (γ) structure near its melting temperature (1536°C). Hence, we choose to calculate the second-shell coordination number (CN_2) in the amorphous state from the ratio between the first- and second-shell coordination numbers in the crystalline f.c.c. structure. This ratio is equal to 2 in a f.c.c. structure, having 12 first-nearest neighbors and six second-nearest neighbors.

2.2. Mechanism of hydrogen diffusion

The above mentioned considerations are used to model the diffusion process of small-volume atoms in an amorphous metal. We assume these atoms to form an extremely dilute solid solution, in which they occupy the octahedral interstitial positions in a f.c.c.-like quasi-lattice. This assumption is based on the similarity between the measured values of diffusion and solubility parameters of hydrogen in amorphous and in f.c.c. metals (see, e.g. Refs [3, 11]). In the case of a f.c.c. lattice there is one octahedral and two tetrahedral interstitial sites per atom. However, we will consider only octahedral positions for interstitial atoms because the volume of the octahedron formed by the atoms of the parent lattice is approximately twice that of the tetrahedron. Now, the diffusion process of atoms of small atomic radius, for example hydrogen, can be described as the result of their jumps over the "sublattice" of octahedral sites. Any tunneling, phonon-assisted or otherwise, is neglected further in our work. Figure 4 presents schematically the location of atoms in such a diffusion process. Atom number 16, located in an interstitial octahedral site, has six first-nearest neighbors (at a distance of $a/2$ from it, where a is the quasi-f.c.c.-lattice parameter) and eight second-nearest neighbors (at a distance of $a\sqrt{3}/2$). Even from the geometric consideration, the position shown as a square in Fig. 4 may be assumed as a saddle-point of a diffusion pass with the smallest value of the diffusion barrier. Thus, it may be assumed that atomic jumps occur mainly across this type of barrier. Such a saddle-point has two first-nearest neighbors (at a distance of $a\sqrt{2}/4$ from it) and four second-nearest neighbors (at a distance of $a\sqrt{6}/4$).

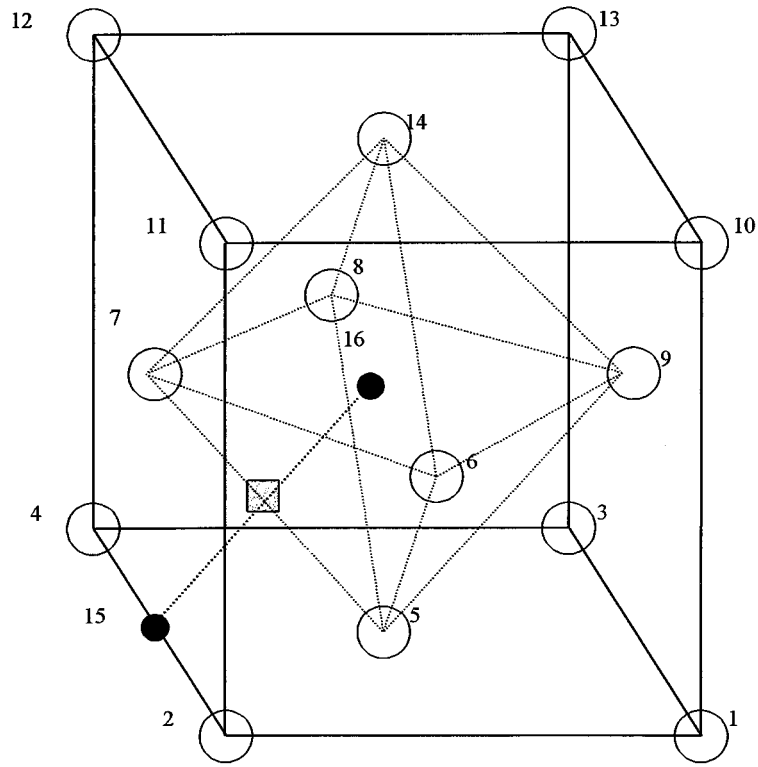

Fig. 4. Schematics of interstitial diffusion of hydrogen atoms in amorphous iron. Empty circles are iron atoms. Filled circles are centers of octahedral interstices. Diffusion of hydrogen is characterized by a jump from position 16 to position 15. The crossed rectangle is the position of the height of the diffusion barrier.

The activation energy for this process may be calculated if the energies of the hydrogen atom in the interstitial position, $\bar{u}_o$, and in the saddle-point, $\bar{u}_p$, are defined. Taking into account only the first- and second-nearest neighbors, we present these energies in the following form [38]:

$$\bar{u}_o = -\left\{\left(1 + \frac{4 \cdot CN_1(T)}{12} + \frac{1 \cdot CN_1(T)}{24}\right) \cdot V_{FeH}(a/2) + \left(\frac{4 \cdot CN_1(T)}{6} + \frac{4 \cdot CN_1(T)}{12}\right) \cdot V_{FeH}(a\sqrt{3}/2)\right\} \quad (4)$$

$$\bar{u}_p = -\left\{\left(1 + \frac{1 \cdot CN_1(T)}{12}\right) \cdot V_{FeH}(a\sqrt{2}/4) + \left(\frac{4 \cdot CN_1(T)}{12}\right) \cdot V_{FeH}(a\sqrt{6}/4)\right\} \quad (5)$$

where CN_1 is the first-shell coordination number and V_{FeH} the interatomic interaction potential between a hydrogen atom and an iron atom at different distances between one another.

In equations (4) and (5), we refer to the first- and second-nearest neighbors around an octahedral interstice and a saddle-point in terms of their position in the quasi-f.c.c.-lattice of amorphous Fe. We choose atom number 5 as the origin atom, thus it is counted as one unit in the calculation of the first-nearest neighbors of the interstitial and saddle-point positions. The contributions of all other kinds of atoms are then expressed in terms of the appropriate temperature-dependent coordination number in the amorphous structure, taking into account the ratio between the first- and second-shell coordination numbers in crystalline f.c.c. structures, as previously explained.

The activation energy for diffusion may now be calculated as

$$\Delta u = |\bar{u}_p - \bar{u}_o|. \quad (6)$$

The diffusion coefficient of hydrogen atoms that are situated in the octahedral interstices of disordered solid solution with f.c.c.-like quasi-lattice may be obtained by substituting this expression into Arrhenius-type formulae:

$$D = D_0 \exp\left(-\frac{\Delta u}{k_B T}\right). \quad (7)$$

Equations (4) and (5) reflect the temperature dependence of the coordination numbers of a quasi-f.c.c. amorphous metal in the vicinity of the "interstitial" impurity. It is easy to see that the activation energy

for the diffusion process becomes temperature-dependent, describing thus the deviation from the Arrhenius law.

2.3. Characterization of the interatomic interactions

For quantitative estimations, the model of interatomic interaction has to be chosen. The Fe–H interaction may be modeled by one of several flexible schemes, including the familiar Lennard–Jones and Harmonic (Hook's law) potentials as well as generalized tabular functions. As follows from simple pseudopotential calculations (see, e.g. Ref. [39] and references therein), the A–B type interaction is repulsive in systems with extremely limited solubility and with no tendencies to intermetallic phase formation. It reflects the tendency for the decomposition of the alloy. To treat the interatomic interactions one may use the perturbation series on potentials in reciprocal space (PSP RS method). It is evident that this approximation will only roughly describe the basic peculiarities of the electronic spectra of solutions. This is especially true for the solutions with transition metals. But as thermodynamic quantities are always obtained as a result of averaging over the spectra, they are less sensitive to its particularities than, for instance, optical characteristics [40]. This is why the PSP RS method can be applied to materials science problems that determine the quantities, which are not too sensitive to details of electron energy spectra of metals and alloys. Making use of the PSP RS method we calculate the Fe–H interatomic interaction potential with simple pseudopotentials. We take into account both electrostatic interactions between ions (unscreened Coulomb interactions) and interactions between the ion cores of the atoms and free electrons. These last interactions are calculated using a pseudopotential approximation based on the screened model potential of Heine and Abarenkov [see Ref. 41]. Parameters of the transition-metal model potential for Fe were taken from Animalu [42]. The results of these calculations are presented in Fig. 5. It should be noted that we consider only very low concentrations of hydrogen (~0.01 at.%) in order to ensure conditions of dilute solid solution and to avoid interactions between hydrogen atoms.

2.4. Hydrogen diffusion in pure amorphous iron

Exploring the effective potential and equations (4) and (5) we may now calculate the activation energy Δu as a function of temperature. Figure 6 presents the Arrhenius plot of the diffusion coefficient of hydrogen in pure amorphous Fe. In this calculation, the value of the frequency factor (D_0) was taken to be $2 \times 10^{-8}\ \mathrm{m^2/s}$, as typical for hydrogen diffusion in amorphous Fe-based alloys [16]. The non-Arrhenius behavior, characterized by a negative curvature of the plot, is clearly evident in Fig. 6. This can be explained by the temperature dependence of the activation energy for diffusion, which results from taking into account the temperature dependence of the local SRO in the metallic glass. This behavior is similar to the one reported by Kirchheim and Stolz [13] for small concentrations and/or high temperatures, when assuming a Gaussian distribution of site energies.

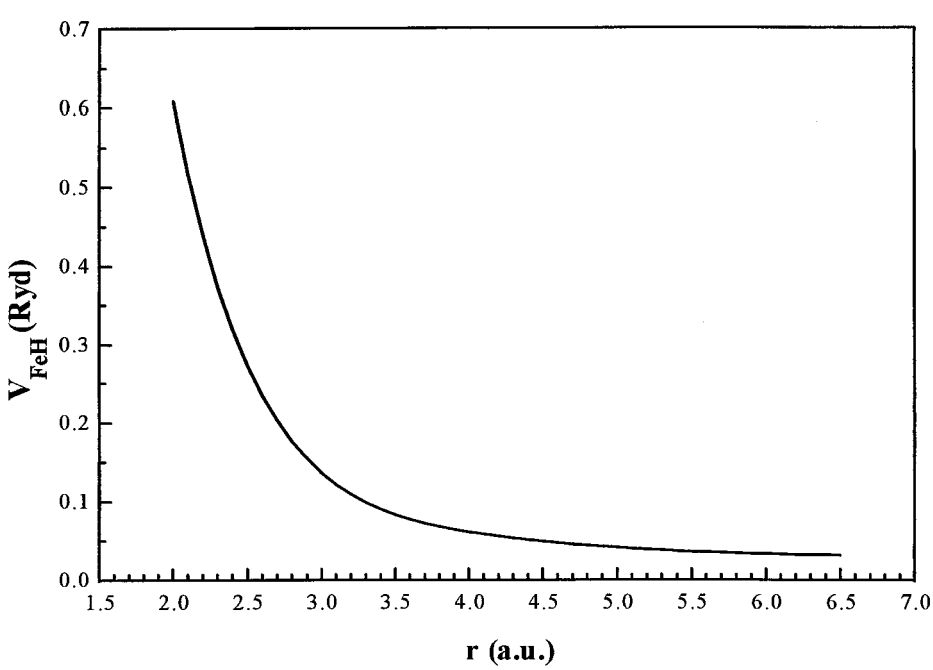

Fig. 5. The effective interatomic interaction potential Fe–H, calculated for extremely dilute Fe–H solid solution [38].

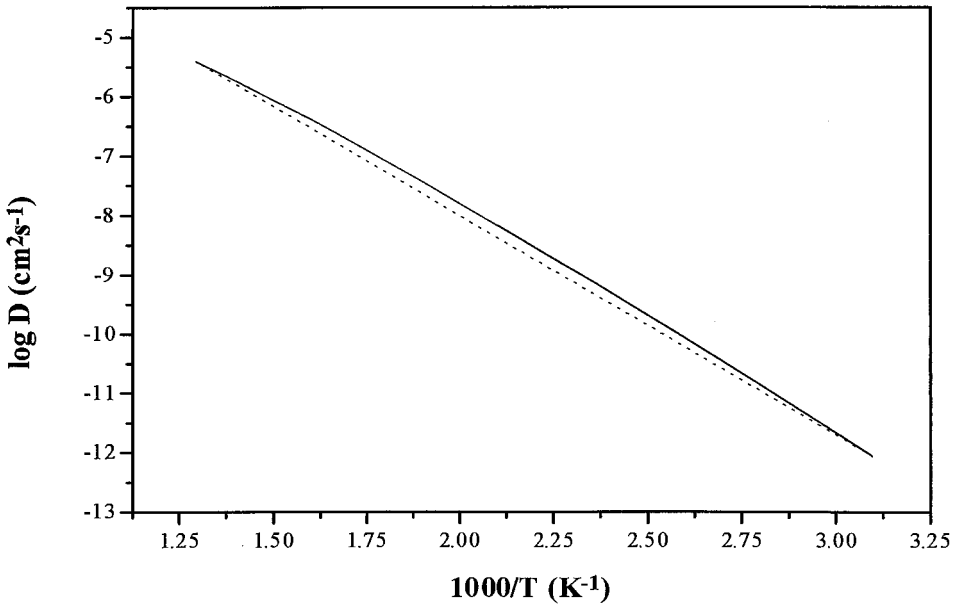

Fig. 6. Arrhenius plot of the diffusivity of hydrogen in pure amorphous Fe. Solid line was calculated using the temperature-dependent activation energy. Dotted line allows the deviation from the linear dependence to be seen [38].

2.5. Hydrogen diffusion in alloyed amorphous iron

In order to study the effect of alloying with silicon or boron on the diffusion of hydrogen in amorphous iron, one has to replace the interatomic interaction potential V_{FeH} in equations (4) and (5) with the effective potential of the complex, $V_{(\mathrm{Fe,Si})\mathrm{H}}$ or $V_{(\mathrm{Fe,B})\mathrm{H}}$.

A formal study of the energy of mixing of ternary alloys based on the PSP RS method is rather difficult. First of all, it is necessary to determine the energy of a disordered multi-component solution and the energy of the standard state. Successive solution of this problem by means of the PSP RS approach should start with presenting the method of electron scattering on the ion component of the alloy and contain the quantities characterizing the presence or absence of ions of some type in the lattice. It is also necessary to determine if the alloying elements occupy the positions of interstices or are substitutes for matrix atoms. In the latter case the problem is much more complicated. Screening functions also have to account for the changes of electron distribution after alloying. These arguments lead to the approach where the probability of electron scattering on the ion in a complex multi-component solution is modeled from the very beginning. With such an approach we shall limit ourselves to merely small concentrations of alloying elements.

The essence of this model is the following. Let us assume that the alloying element atoms substitute the solvent atoms. It is evident that these impurity atoms will result in a change of the electron spectrum. Let us consider that the system still has almost free electrons, which are scattered on the atoms located in the solvent lattice nodes, using the model of a virtual crystal. Now, several factors affecting the interatomic interaction potential may be corrected according to

$$\omega = \sum_{i=1}^{n} c_i \omega_i \tag{8}$$

where ω_i denotes the probability of electron scattering on an ion of sort i (either iron or an alloying element ion), the mean volume per atom, the valence or the mean deviation from the valence of this ion, n the number of different sorts of ions in the lattice sites, and c_i are concentrations of these sorts of ions in the lattice. This formula is derived from applying the coherent potential approximation (CPA) for the electron scattering probabilities [26, 27] under conditions of absolute disordered solution. With respect to the mean volume per atom, this approximation also seems applicable because of extremely small concentrations of alloying elements, simply representing Zen's law for extremely dilute solutions. Parameters for silicon and boron were taken for calculations from Refs [41, 42]. Using this procedure it was found that the interatomic interaction potential increases as a result of alloying iron with either silicon or boron.

Results of the calculation of the activation energy of hydrogen diffusion in amorphous iron are presented in Fig. 7 vs temperature for different concentrations of alloying element. The dependence of the activation energy on temperature may be noticed again. In addition, the activation energy increases significantly as a result of alloying with either sili-

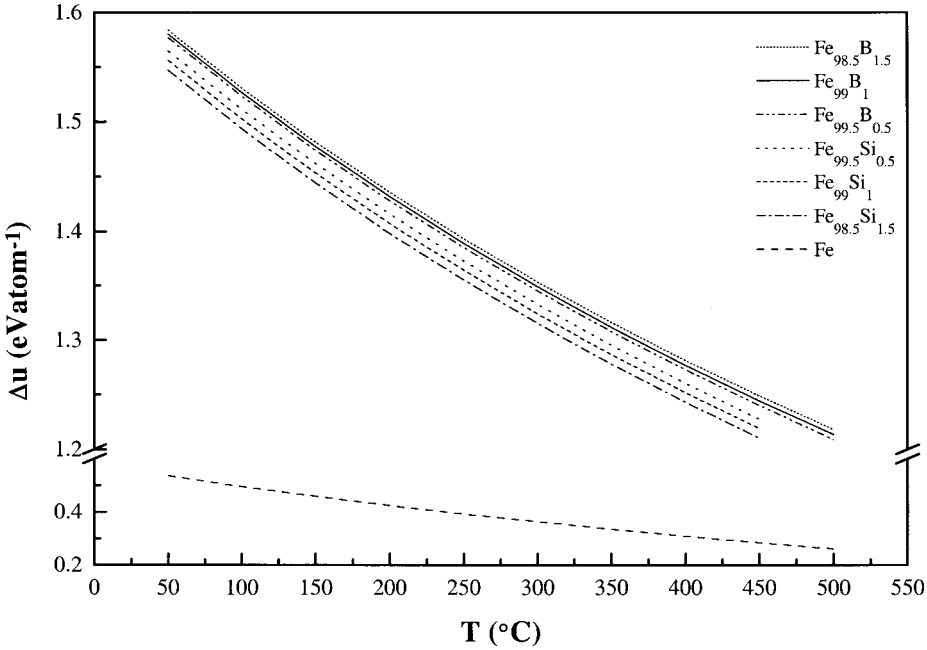

Fig. 7. The activation energy of hydrogen diffusion in amorphous Fe vs temperature and concentration of alloying elements.

con or boron. At these relatively low concentrations (0.5–1.5 at.%) of the alloying element, silicon and boron have similar influence on the activation energy, though boron increases it slightly more. It should be noted, however, that at higher concentrations (4.0–9.5 at.%) of alloying elements an opposite tendency was observed, silicon having a more pronounced influence. Any fundamental explanation of this behavior should take into account the effect of alloying on the structure through changes in the density and radial distribution functions. In the absence of experimental data on the dependence of these functions on the composition of the amorphous Fe-based alloy, we suggest a semi-qualitative explanation.

The activation energy may be affected by the mean volume per atom and the effective number of free electrons of the alloying element, compared to iron. Reducing the mean volume per atom (e.g. by alloying Fe with B) should lead to a decrease in the mean quasi-lattice parameter. Consequently, the distance between a hydrogen atom in an interstitial site or a saddle-point and its neighboring metal/metalloid atoms decreases, thus increasing the activation energy of diffusion. Similarly, alloying of iron with silicon should lead to a decrease in activation energy. However, there is also a correlation between the electronic structure of the impurity ion and hydrogen solubility or diffusivity. According to Weinstein and Elliott [43], an element having a larger number of free electrons in comparison to pure iron ($n_{\mathrm{eff}} > -2.66$) is expected to decrease the solubility of hydrogen in pure liquid iron. From the relationship between the thermodynamic functions of a solute and its mass flow with temperature and composition [44] we may expect such an element to decrease the diffusivity of hydrogen in iron as well. Thus, alloying with silicon or boron is expected to lead to an increase in the activation energy of diffusion. On the basis of our results we may conclude that as the concentration of silicon or boron increases, the effect of the effective number of free electrons on the activation energy becomes more significant than the effect of the mean volume per atom. It should be mentioned that the results obtained using our model are, in general, in accordance with the experimental results reported elsewhere. Gibala [44] found that alloying with silicon decreases both the solubility and diffusivity of hydrogen in either crystalline or liquid iron. The effect of the alloying element on hydrogen diffusivity is explained in that work in terms of the interaction between hydrogen and solute atoms, leading to an increase in the jump time of hydrogen. Similar results are presented in the works of Geller and Sun [45] and Riecke *et al.* [46]. Finally, Smialowski [47] reports that boron slows the permeation of hydrogen through iron.

3. CONCLUSIONS

1. Hydrogen diffusion in metallic glasses is characterized by a non-Arrhenius behavior. This deviation from the Arrhenius behavior may be related to the temperature dependence of the SRO in the amorphous structure. The latter

enters the activation energy in a natural way by means of coordination numbers, which appear to vary with temperature.

2. The diffusion process of hydrogen in amorphous metals may be well described by means of a f.c.c.-like quasi-lattice. It is important to identify the first- and second-nearest neighbors around an interstitial site and a saddle-point in terms of their position (appropriate atomic shell) in this quasi-lattice.
3. Alloying of amorphous iron with silicon or boron significantly increases the activation energy of hydrogen diffusion. This increase may be partially explained in terms of the mean volume per atom and the electronic structure of the alloying element.
4. The simple model presented in this paper may be used to study the tendencies in the diffusion behavior in metallic glasses under alloying, instead of using complicated and time-consuming Molecular Dynamics or Monte-Carlo simulations. The temperature dependence of activation energy may influence also the other mechanisms of mass transfer in amorphous metals, for example the tunneling or phonon-assisted transport of light (hydrogen) atoms.

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