



SDI Review Form 1.6

PART 1:

Journal Name:	British Journal of Applied Science & Technology
Manuscript Number:	2013_BJAST_3788
Title of the Manuscript:	Local Structure and Tracer Diffusion Mechanism in Amorphous Fe-based Alloys

General guideline for Peer Review process is available in this link:

(<http://www.sciencedomain.org/page.php?id=sdi-general-editorial-policy#Peer-Review-Guideline>)

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PART 2: Review Comments

	Reviewer's comment	Author's comment (if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)
Compulsory REVISION comments	1. The present manuscript is an extension of the earlier work (Ref.20) which was co-authored by the present author. The model incorporates a number of parameters. The success of the model depends upon the numerical values given to the parameters. A more complete discussion on the justification for values of the parameters used here should be given. For example, a value $10^{12}/\text{sec}$ used appears too high for amorphous solid which is closer to the value for crystalline solid. Further, the vibration frequency of iron and boron atoms may not be the same. 2. Arrhenius plot of diffusivity should be non-linear if the more one diffusing species are involved in the process of diffusion. 3. Author considers two types of two types of relaxation processes-one with $\text{dr} = 0.4\text{\AA}$ and another one with $\text{dr} = 0.02\text{\AA}$. He should clarify in what way they differ and what are activation energies associated with two processes. 4. With respect to the potential energy diagram in Fig.4, author states that the barrier heights for bubble splitting may vary from 0.6eV to 3.2 eV. In this context, it should be noted that any potential barrier larger than a few tenth of electron volts cannot be crossed via thermal	1. Atoms in simulation model are described as hard spheres and non-conductive. This means that the vibration frequency of iron and boron atoms is not interested in model. The Pak-Doyama-type pair potentials were chosen for all atomic pairs in the system, because they were successfully used for the construction of the models of the transition metal-metalloid alloys. Further, using the Pak-Doyama pair potential has obtained a good correspondence with experimental radial distribution functions for our simulation models. 2. In this study, I only consider the temperature dependence follows Arrhenius behavior for model M_1, which consisting Fe atoms. This model composed of only one type of atom. 3. Model was prepared by relaxing with a statistic relaxation (SR) step length of $0.4\text{\AA}$, this process is like shaking many times the atomic arrangement in model. Then we relax the obtained model with the SR step length $0.01\text{\AA}$ to reaches a new equilibrium. 4. As mention in ref. [21], the energy barrier is determined by the difference between the maximum point in the potential energy profile (PEP) and the site energy of the diffusion atom. Hence, the barrier heights of diffusion atom in bubbles splitting may vary



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	activation in the temperature ranges where metallic glasses are exist in a metastable state. 5. According to the author, single vacancies are unstable in an amorphous matrix. However, experimental evidence exists which supports diffusion via single vacancies as in the case of crystalline solids.	from 0.6 to 3.2 eV. 5. As described in manuscript, an atom on surface of bubbles (single-vacancy) move into bubbles centre lead to diffusion of neighboring atoms, present bubbles disappear and a other bubbles appears in somewhere in matrix, it would be not position of the previous moving atom. So, bubbles play role as vacancy in crystalline. However, the diffusion mechanism via bubbles is not like vacancy in crystalline, where the position of moving atom is created a new vacancy. Note that the number of bubbles weakly depends on temperature, but very sensitive to the relaxation degree.
<u>Minor</u> REVISION comments	The language (specifically, the grammer) of the needs to be reviewed and suitably revised. The word "simplex" has been used to describe a collection atom on a circum-sphere (CS). I think the word "complex" should be used instead.	I think the work "complex" could use to describe cluster of atoms in my simulation model.
<u>Optional/General</u> comments	The authors should be encouraged to respond to comments made here.	