Iron phosphate glasses: Structure determination and displacement energy thresholds, using a fixed charge potential model

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**Abstract**

Iron phosphate glass is a versatile matrix for the immobilisation of various radioactive elements found in high-level nuclear waste (HLW). Quenched glass structures of iron phosphate glasses with Fe/P ratios of 0.33, 0.67 and 0.75 and with a composition of 40 mol% Fe₂O₃ and 60 mol% P₂O₅, with 4% and 17% Fe²⁺ ion concentrations were generated using molecular dynamics and the threshold displacement energies calculated. In the minimum energy structures, we found that in nearly all cases the P atoms were 4-fold coordinated. The potential energy per atom increased with increasing concentration of Fe²⁺ ions with similar Fe/P ratio, suggesting that decreasing the Fe³⁺ content is a stabilising factor. The average bond distances between Fe²⁺–O, Fe³⁺–O, P–O and O–O were calculated as 2.12, 1.88, 1.5 and 2.5 Å respectively. The threshold displacement energy (E₉) was found to be dependent upon the ion specie, less for Fe³⁺ ions compared to Fe²⁺ ions, and was overall slightly lower than that determined for borosilicate glass.

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1. Introduction

Phosphate glasses, due to their favourable properties such as: reasonably low liquid and glass transition temperatures, low viscosity, high thermal expansion coefficient, high electrical conductivity and high ultraviolet transmission, find application in a wide range of fields. For example, phosphate glasses are used in lasers [1], solid electrolytes [2], bio-medical devices [3] and nuclear waste immobilisation [4]. A good review up to the year 2000 is given in [5]. According to the literature [6], in spite of the good glass forming characteristics of phosphate glasses, their relatively poor chemical durability limits their application, especially in the field of nuclear waste immobilisation. However, a new group of phosphate glasses, iron phosphate glass, is being considered as a promising matrix for the immobilisation of high-level nuclear waste (HLW). Quenched glass structures of iron phosphate glasses with Fe/P ratios of 0.33, 0.67 and 0.75 and with a composition of 40 mol% Fe₂O₃ and 60 mol% P₂O₅, with 4% and 17% Fe²⁺ ion concentrations were generated using molecular dynamics and the threshold displacement energies calculated. In the minimum energy structures, we found that in nearly all cases the P atoms were 4-fold coordinated. The potential energy per atom increased with increasing concentration of Fe²⁺ ions with similar Fe/P ratio, suggesting that decreasing the Fe³⁺ content is a stabilising factor. The average bond distances between Fe²⁺–O, Fe³⁺–O, P–O and O–O were calculated as 2.12, 1.88, 1.5 and 2.5 Å respectively. The threshold displacement energy (E₉) was found to be dependent upon the ion specie, less for Fe³⁺ ions compared to Fe²⁺ ions, and was overall slightly lower than that determined for borosilicate glass.

The iron phosphate glass with the composition 40 mol% Fe₂O₃–60 mol% P₂O₅ (IPG), has been reported by various researchers to have different ratios of Fe²⁺/Fe [7,12,24,25]. The concentration of Fe²⁺/Fe in glass with the same atomic composition varies from 4 to 20%, while the density varies between 2.9 and 3.0 g cm⁻³ with the uncertainty in density ranging from ± 0.005 to 0.02 g cm⁻³ [7,24]. The concentrations of Fe²⁺/Fe and density of IPG reported by us [12] were 4% and 2.9 g cm⁻³ respectively. The promising composition of 40 mol% Fe₂O₃–60 mol% P₂O₅ (IPG) is found with the varying density depending on the concentration of Fe²⁺ in the glass. It is evident from the literature [7,24,25] that as the concentration of Fe²⁺ in IPG increases, the density also increases for the same atomic composition. It has been shown experimentally by Mössbauer spectroscopy [24], that as the melting temperature of IPG increased from 1423 to 1673 K, the density of the glass increased along with the increase in concentration of Fe²⁺. Thus, it becomes essential to model the structure of iron phosphate glasses specific to the composition and Fe²⁺/Fe ratio.

**Keywords:**
Iron phosphate glass; Computer simulation; Structure; Displacement energy thresholds
It is well known that amorphous structures are more difficult to handle computationally than crystalline lattices since many different atomic configurations are possible. Therefore averaging over many different structures is very important. It is also essential to have good inter-atomic potentials that describe the amorphous systems. A recent paper [21] reported one of the first studies of iron phosphate glasses using fixed charge potentials.

Other authors have also developed potentials of a form that could be used to model phosphate glasses. However potentials that involve shell models such as that by Ainsworth et al. [26] are not really suitable for radiating systems. However potentials that involve shell interactions between ionic charges.

For example, the Stillinger–Weber potential (Eq. (1)) to the ZBL potential using a splining function. The Stillinger–Weber potential was chosen because the cos(θ) term is obtainable directly from the atomic separations via the dot product (also, the derivatives are a function of cos(θ)). The Stillinger–Weber potential has continuous derivatives and a built-in smooth cut-off to zero at r = r0. We fit the Stillinger–Weber potential to the original authors' function by computing the parameter λ. We do this by computing the Taylor series expansion of Eq. (2) at θ = θ0 to the second order. For this calculation we set γ = 0.5 eV and rj = rk = 1.5 Å (the equilibrium bond length).

For both triplets (P–O–P and O–P–O), we set this equal to the original authors' function and rearrange to find λ. These parameter values (λ, γ and θ0) for both triplets are summarised in Table 1.

For radiation damage studies, the two-body potential cannot model the repulsion between nuclei when the inter-particle separation is small. A screened Coulomb potential is normally used to model such interactions and the ZBL model [33] is the commonly used model when the separation is small. As a result we have joined the two-body potential given in Eq. (1) to the ZBL potential using a splining function. The details and parameters for the splining function are given in Table 2.

Each of the glass structures was prepared by distributing the required number of atoms of each species randomly within a cubic box. We then use a simple temperature-rescaling algorithm [34] to quench the system. This works by measuring the temperature at each time-step. If the temperature exceeds the desired value by 7%, then, the velocities of all the atoms are rescaled, such that, the temperature is the desired value. We quench the system from 6000 K to 10 K at a rate of the order of 10000 K/s.

Table 1

| Interaction | a (Å) | b (Å) | c (Å) | d (Å) | e (Å) | f (Å) | g (Å) | h (Å) | i (Å) | j (Å) | k (Å) | l (Å) | m (Å) | n (Å) | o (Å) | p (Å) | q (Å) | r (Å) | s (Å) | t (Å) | u (Å) | v (Å) | w (Å) | x (Å) | y (Å) | z (Å) |
|------------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| Fe2+–O     | 1.1  | 1.9  | 38.456891 | 115.889467 | 166.591541 | 122.352450 | 44.173231 | 6.208431 |
| Fe2+–P     | 0.9  | 1.9  | 11.672255 | 14.838923 | 17.690051 | 15.321189 | 6.858104 | 1.470608 |
| Fe3+–O     | 0.2  | 0.85 | 11.274280 | 21.323242 | 44.020565 | 69.570862 | 60.519843 | 21.948215 |
| Fe2+–P     | 0.7  | 1.45 | 13.468001 | 28.411311 | 49.821000 | 53.364231 | 28.581882 | 5.844285 |
| Fe3+–P     | 0.9  | 1.9  | 12.389419 | 20.647793 | 60.460856 | 30.341842 | 10.171431 | 1.285723 |
| Fe3+–O     | 0.5  | 1.25 | 13.468076 | 36.254018 | 82.396027 | 109.951757 | 74.401925 | 20.16820 |
| Fe2+–O     | 0.4  | 1.45 | 13.468076 | 36.254018 | 82.396027 | 109.951757 | 74.401925 | 20.16820 |
| O–P        | 0.25 | 1.38 | 9.273627 | 11.581100 | 8.397094 | 2.457030 | 0.030643 | 0.993801 |
| P–O        | 0.25 | 1.03 | 11.160800 | 26.912807 | 75.616106 | 136.539861 | 112.56770 | 36.456113 |
| P–P        | 0.24 | 1.26 | 11.026363 | 16.858035 | 23.118958 | 21.054756 | 11.153372 | 2.724575 |
The composition of each atom (in atomic %) of iron phosphate glasses at the optimum density for the systems containing the larger number of atoms.

| Glass system | ρ (g cm⁻³) | CN | Fe²⁺ at.% | Fe³⁺ at.% | P at.% | O at.% |
|--------------|-----------|----|-----------|-----------|-------|-------|
| Fe₃(PO₄)₂ | 3.2 | 1 | - | - | 3.17 |
| Fe₄(PO₄)₃ | 3.04 | 1 | - | - | 4.06 |
| Fe₅(PO₄)₃ | 3.04 | 1 | - | - | 11.08 |
| Fe₆(PO₄)₃ | 3.04 | 1 | - | - | 57.23 |

CN: coordination number.

3. Results and discussion

The details of the composition of the smaller systems of iron phosphate glass, Fe/P atomic ratio and the number of atoms quenched are given in Table 3. Fig. 1 shows the average potential energy obtained as a function of glass density for systems Fe₃(PO₄)₂, Fe₃(PO₄)₃, and Fe₄(PO₄)₃. The composition of 40 mol% FeO₃–60 mol% P₂O₅ is the same as that of the Fe₄(PO₄)₃ glass and can also be referred as Fe₃(P₂O₇)₂ glass respectively. The lowest energy structure of Fe₃(PO₄)₂ glass (containing both Fe²⁺ and Fe³⁺ ions) had a higher density compared to the other systems containing only Fe³⁺ ions. Larger systems of Fe₃(PO₄)₂ and Fe₆(PO₄)₃ were generated with the density that showed the lowest energy in the smaller atom systems. The computation was done a minimum of three times for each large system at the fixed density. Whenever the difference in energy between the structures was small (<1%), the structure with the lowest potential energy was chosen for further analysis based on certain logical guidelines.

The logical guidelines used to choose the best structure when the difference in potential energy was small are given below:

1. The coordination of P should be 4 for a maximum number of P ions in the glass.
2. The coordination of Fe²⁺ and Fe³⁺ varies between 4 and 6. The structures that contain iron ions with a coordination number of 3 are less stable.
3. The coordination number of oxygen varies between 1 and 3. The more stable structures have the maximum number of oxygen ions with coordination number 2.

For Fe₅(PO₄)₃ glass (130 atoms), the difference in potential energy between the structures with densities of 2.9 and 3.04 g cm⁻³ was very small, i.e., 3.5 × 10⁻³ kJ/mol. Thus larger systems were modelled using both the densities (2.9 and 3.04 g cm⁻³) for Fe₅(PO₄)₃ glass (1300 atoms). For Fe₆(PO₄)₃ glass (1300 atoms), based on the guidelines above, the structure with a density of 3.04 g cm⁻³ was chosen for...
The coordination of ions within the Fe$_3$(P$_2$O$_7$)$_2$ glass structure.

Before describing the results of the simulations, it is useful to understand the experimental observations on crystallisation of iron phosphate glasses. Iron phosphate glass crystallises to FePO$_4$, Fe$_2$(P$_2$O$_7$)$_3$, Fe$_3$(P$_2$O$_7$)$_2$, Fe$_4$(P$_2$O$_7$)$_3$ and Fe$_2$P$_2$O$_7$ depending on the composition, atmosphere of crystallisation and ratio of Fe$^{2+}$/Fe$^{3+}$ [11,37]. In order to compare the structures, the potential energy per atom was determined and this is presented in Fig. 3. The potential energy per atom increases linearly with the Fe/P ratio. This plot also clearly shows that as the concentration of Fe$^{2+}$ ions increases in the glass, the potential energy per atom also increases.

In the experiment, the starting material contains only Fe$^{3+}$ ions but during the preparation process, some Fe$^{2+}$ ions form. Ammonium dihydrogen phosphate is used as the source of phosphorus during the preparation of the iron phosphate glass. Evolution of ammonia, a reducing agent, during the preparation of the iron phosphate glass (due to the decomposition of ammonium di-hydrogen phosphate), reduces some Fe$^{3+}$ to Fe$^{2+}$. However, the reducing effect can be minimised by a low temperature pre-calcination, as indicated in ref. [40]. Hence the most stable structure would be expected to be the one with the lowest concentration of Fe$^{3+}$ ions, that is the IPG containing 4% Fe$^{3+}$ concentration.

Modelling studies on the structure of iron phosphate glasses are given in refs. [21,22]. During the structural evolution of the IPG, Stoch et al. reported [22] the formation of crystallised products in air as

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**Table 5**

| System (IPG) | Contribution (%) | Fe$^{2+}$/Fe$^{3+}$/P/O at.% | Fe/P atomic ratio |
|--------------|------------------|-------------------------------|------------------|
| Fe$_2$(P$_2$O$_7$)$_3$, Fe$_3$(P$_2$O$_7$)$_2$, Fe$_4$(P$_2$O$_7$)$_3$ | Fe$_2$P$_2$O$_7$ | 4% Fe$^{2+}$ | 14 | 12 | 74 | 0.51 | 12.24 | 19.53 | 67.71 | 0.65 |
| | | 17% Fe$^{2+}$ | 54 | 10 | 36 | 2.27 | 11.0 | 19.41 | 67.31 | 0.68 |
FePO₄ and Fe₂P₂O₇. Though the starting composition was 40 mol% Fe₂O₃, the final crystallised products contain Fe/P with an atomic ratio of 1, regardless of the contribution of each phase (FePO₄ and Fe₂P₂O₇) in the glass. The Fe/P ratio increases after crystallisation, indicating the loss of P and O. This can be explained as follows:

$$40 \text{ mol} \% \text{ Fe}_2\text{O}_3 – 60 \text{ mol} \% \text{ P}_2\text{O}_5 = \text{Fe}_2\text{P}_2\text{O}_{21} \text{(amorphous)}$$

The calculated elastic properties (bulk modulus and shear modulus) of IPG containing 4% and 17% concentrations of Fe²⁺ ions are presented in Table 8. The values of these properties are obtained as the average of the three methods employed in GULP [30]. Experimentally determined bulk modulus and Young’s modulus of IPG with a composition of 40 mol% Fe₂O₃–60 mol% P₂O₅ were 47 GPa and 70–72 GPa respectively as reported in the literature [19,23,42-44] for iron phosphate glasses. Table 7 presents details of the mean bond distance between Fe²⁺ ions and O in the iron phosphate glasses that we have modelled.

Eq. (4) also justifies the formation of Fe²⁺ ions (Fe₂P₂O₇) from the starting composition containing only Fe³⁺ ions with the loss of oxygen. Thus some Fe²⁺ are to be expected despite the fact that the model gives a higher cohesive energy when the amount of Fe²⁺ is minimised.

The radial distribution functions of Fe₃(P₂O₇)₂ glass and IPG containing 4% Fe²⁺ concentration are shown in Fig. 4. The bond distance between Fe³⁺–O is shown in Table 8. The values of these properties are obtained as the average of the three methods employed in GULP [30]. Experimentally determined bulk modulus and Young’s modulus of IPG with a composition of 40 mol% Fe₂O₃–60 mol% P₂O₅ were 47 GPa and 70–72 GPa respectively as reported in the literature [45,46]. The calculated properties are in good agreement with the experimentally reported values.

Table 7

| Glasses | Mean bond distance (Å) |
|---------|------------------------|
| Fe³⁺–O  | Fe²⁺–O                 |
|         | (2.08–2.12)            | (1.89–1.91)   |
| P–O     | (1.48–1.55)            |

Fe₃(P₂O₇)₂ 2.07 1.87 1.5
Fe₄(P₂O₇)₃ – 1.87 1.5
Fe₅(P₂O₇)₄ 1.89 1.5
IPG with 4% Fe²⁺ 2.12 1.88 1.5
IPG with 17% Fe²⁺ 2.12 1.88 1.5

* The values in parentheses are experimental values from refs. [19,35–38].
the ion in IPG. Fig. 6 gives $E_d$ for ions of fixed coordination in IPG containing both 4 and 17% concentrations of Fe$^{2+}$ ion. It is clear from the plots that $E_d$ varies depending on the nature of the ion with the lowest values for the Fe$^{2+}$ ions. However, similar values of $E_d$ were observed for IPG containing both 4% and 17% concentrations of Fe$^{3+}$ ions. This indicates that $E_d$ does not change with the concentration of Fe$^{2+}$ ions in IPG but as shown in Fig. 6, Fe$^{2+}$ has a lower $E_d$ than Fe$^{3+}$.

Since phosphorous is 4-fold coordinated in all the iron phosphate glasses, the values of $E_d$ for phosphorous ions in all these glasses are compared and shown in Fig. 7. It is apparent from the plot, that $E_d$ remains similar for phosphorous ions in all the iron phosphate glasses. The peak values of $E_d$ of the different ions as a function of their coordination number are presented in Table 9. Although a large number of calculations were performed to determine these values, there is a wide statistical variation, and the values for a given species are very similar for the different coordination numbers.

The values of $E_d$ for the O ions given in Table 9 are very similar to those calculated for the borosilicate glasses [34] but the thresholds for P and Fe$^{2+}$ are lower than those calculated for boron and silicon suggesting that the phosphate glasses might not be as radiation resistant as the borosilicate.

### 4. Conclusion

The structures of iron phosphate glasses with varying Fe/P atomic ratios were modelled as a function of density using the molecular dynamics simulation method. Furthermore, the structures of iron phosphate glass with a composition of 40 mol% Fe$_2$O$_3$–60 mol% P$_2$O$_5$ (IPG) containing the concentrations of 4 and 17% Fe$^{2+}$ ions, were also computed and compared in order to understand the effect of Fe$^{2+}$ concentration. The potential energy per atom of all these glasses indicated that the system energy increases with both increasing Fe/P atomic ratio and Fe$^{2+}$ concentration. The computed elastic properties of

| Glass   | Bulk modulus (GPa) | Shear modulus (GPa) | Young’s modulus (GPa) |
|---------|--------------------|---------------------|-----------------------|
| IPG, 4% Fe$^{2+}$ | 48                 | 31                  | 81                    |
| IPG, 17% Fe$^{2+}$ | 44                 | 31                  | 71                    |
40 mol% Fe$_2$O$_3$–60 mol% P$_2$O$_5$ glass were found to be similar to that of the experimental values reported in the literature. The threshold displacement energy varies with the nature and as well as with the coordination of ions in these iron phosphate glasses. However, similar threshold energies were obtained for IPG containing 4 and 17% Fe$^{2+}$ ions. The threshold energy of phosphorous ions remains the same for all the iron phosphate glasses. The results show that the peak displacement energy threshold of the Fe$^{3+}$ ions is lower than that for Fe$^{3+}$ and O ions. The cohesive energy of the glasses is also reduced as the amount of Fe$^{2+}$ increases. This suggests that for the purposes of nuclear waste immobilisation, it would be preferable to produce the glasses with as low a Fe$^{2+}$ content as possible. This is not the only consideration since the glasses must also be suitable to incorporate heavy atoms such as caesium and the associated structure is also important. However, the bond lengths and densities have been shown to vary only slightly as a function of composition.

Future work will investigate the structural changes induced by collision cascades in the glasses. It was for this purpose that the modified potential was developed since it provides a better description of the collision dynamics than the simple Teter model developed only for structural studies.

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