Theoretical approach to the Poisson's ratio behaviour during structural changes in metallic glasses

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Abstract

Recently, various studies dealing with the relationship between the elastic constants and various of the macroscopic properties of metallic glasses have been published. Particularly, the correlations between the Poisson's ratio of the glass and both the super-cooled liquid viscosity behaviour and the brittle-ductile transition have aroused much interest. In this work, we use a model developed by Knuyt et al. (1990 and 1991) based on a Gaussian distribution for the nearest-neighbour distance in an ideal uni-component metallic glass, in order to describe qualitatively the dependence of the Poisson's ratio on changes of the atomic structure. The results are used to explain the experimental results obtained in structural relaxation and hydrostatic pressure tests of metallic glasses.

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I. INTRODUCTION

The elastic properties of a glass determine many of its mechanical qualities. Besides, the change of the Bulk (K), Shear (G) and Young (E) moduli under pressure or temperature treatments gives information of the changes in the atomic structure of the glass. The interatomic forces and the structure of a liquid or a glass determines its vibrational properties and hence its elastic constants. The values of the elastic constants K, G, E and the Poisson's ratio, ν, can be obtained experimentally by many methods in solids, such as mechanical deformation or sound wave propagation. For liquids, the instantaneous elastic constants can be obtained from velocity measurements of high-frequency sound waves in order to avoid contributions of fast structural relaxations.

A glass inherits its structure from the liquid. The structural state of the glass is described in terms of the fictive temperature T_f. It is known that metallic glasses become stiffer during structural relaxation, K, G and E increase if T_f decreases[1][2][3]. Similarly, it is expected that the instantaneous K, G and E increase as temperature decreases in an equilibrium liquid. In hydrostatic pressure tests upto 0.5GPa the elastic moduli K, G, and E are also found to increase as pressure increases[4][5][6]. The density of the glass ρ increases in both processes, that is when lowering T_f and increasing pressure. This explains the increase in K, G and E as interatomic distances become smaller. However, the Poisson's ratio of metallic glasses exhibits different behaviour in each case; ν decreases after structural relaxation[3] but increases under pressure[4][5] [6]. The Poisson's ratio is directly related to the bulk and shear modulus ratio and it can be calculated as

$$\nu = \frac{1}{2} - \frac{3}{(6K/G) + 2}. \tag{1}$$

Although in both processes the glass becomes denser, the opposite behaviour of K/G of a metallic glass when lowering T_f and when increasing pressure indicates a very different change of the structure.

Recently, a rough correlation between the fragility parameter of the supercooled liquid and the K/G of the corresponding glass was noticed for chemically different glasses[7]. The fragility parameter of a liquid indicates the grade of departure of the viscosity $\eta(T)$ from the Arrhenius equation. This latter correlation would imply a general relationship between elastic properties and the structural relaxation behaviour of liquids near glass transition,

which would be of practical interest in the selection of alloying components for bulk metallic glasses design[8].

In the following sections we use a theoretical model developed by Knuyt et al.[9][10][11] to describe qualitatively the structural changes responsible of the Poisson's ratio behaviour described above. The model is based on a Gaussian distribution approach for the nearest-neighbour atomic distance in an ideal uni-component metallic glass.

II. THEORY

The approach made by Knuyt et al.[9][10][11] is based on the assumption of a Gaussian radial distribution function $RDF\,(r)$ for the atomic positions in an amorphous metal. This RDF is defined by a mean position r_i and a width σ_i for the atoms in a given i-shell around a central atom

$$RDF\,(r) = \frac{r}{(2\pi)^{\frac{1}{2}}} \sum \frac{N_i}{r_i \sigma_i} \left(\exp\left[-\frac{(r-r_i)^2}{2\sigma_i^2} \right] - \exp\left[-\frac{(r+r_i)^2}{2\sigma_i^2} \right] \right) \tag{2}$$

where N_i is the number of atoms in the i-shell. This RDF gives a good approach to the experimental pair correlation functions found in amorphous metals[12]. The model assumes that the elastic properties are determined by the immediate surroundings of the atoms. Specifically, contributions of the atomic configuration further than the first shell, that is out of the range of the interatomic potential, are not taken into account. Therefore, the calculations are based on an approximated RDF corresponding just to the first shell, which can be written as

$$RDF\,(r) = \frac{r}{(2\pi)^{\frac{1}{2}}} \frac{N_1}{r_1 \sigma_1} \left(\exp\left[-\frac{(r-r_1)^2}{2\sigma_1^2} \right] \right), \tag{3}$$

where the parameters determining the shape of the distribution are r_1 and σ_1. From this RDF function, expressions in terms of r_1 and σ_1 can be calculated for the atomic volume and coordination number distributions of the glass, and for the interference function which would be obtained in diffraction experiments. For details see ref. [9].

For the calculation of macroscopic properties, Knuyt et al. chose an interatomic potential with harmonic and anharmonic terms written as

$$U\,(r) = a\,(r-r_m)^2 + b\,(r-r_m)^3 \tag{4}$$

where $a > 0$, $b < 0$ and r_m is the position of the minimum. The important region of this potential concerning the RDF of equation (3) is within the interval $r_m - \sigma_1 < r < r_m + \sigma_1$. Estimated values for a, b, and r_m corresponding to real amorphous metals give $r_m + \sigma_1$ well below the position of the maximum at $r_m - 2a/3b$, which can be considered the cut-off distance for the potential. This potential is chosen instead of a more realistic and complex one for the sake of simplification in further calculations.

Using the approximated RDF and the interatomic potential of equations (3) and (4), Knuyt et al. performed semi-quantitative analysis of various macroscopic quantities such as the relaxation energy, and the change in the atomic volume and viscosity during relaxation of amorphous metals. A good agreement with the experimentally observed behaviour was found when introducing realistic values for the interatomic potential and values of r_1 and σ_1 obtained from experimental diffraction data.

A. Calculation of the elastic constants for an amorphous metal

Following Knuyt et al.[11] the calculation of the bulk and the shear moduli is performed assuming two-particle pair interactions. Supposing we know the positions $\mathbf{r}_k$ of any atom k in an amorphous material and the interatomic potential $U(|\mathbf{r}_k - \mathbf{r}_{k'}|)$, the total energy of the system is given by

$$E_{tot} = \frac{1}{2} \sum \sum_{k \neq k'} U\left(|\mathbf{r}_k - \mathbf{r}_{k'}|\right) \tag{5}$$

the sum running over all the atoms of the system. In the case of a uniform bulk deformation the position of a k atom is given by

$$\mathbf{r}_k = \mathbf{r}_k^0 + \varepsilon \mathbf{r}_k^0 \tag{6}$$

where $\mathbf{r}_k^0$ is the initial position in the undeformed situation and ε is a small number. Substituting the previous equation into the energy equation (5) and expanding in Taylor series upto second order one obtains

$$E_{elastic,bulk} = \frac{\varepsilon^2}{4} \sum \sum_{k \neq k'} \left(r_{kk'}^0\right)^2 U''\left(r_{kk'}^0\right) \tag{7}$$

where

$$r_{kk'}^0 = \left|\mathbf{r}_k^0 - \mathbf{r}_{k'}^0\right|. \tag{8}$$

$E_{elastic}$ is the energy increase in the system due to the deformation, the first term in the Taylor expansion has to be zero as the material must have the lowest energy for the undeformed state $\varepsilon = 0$. On the other hand, the general expression for the elastic energy in a stressed material is

$$\frac{E_{elastic}}{V} = \frac{1}{2}\sum_{i=1}^{6}\sum_{j=1}^{6} C_{ij} e_i e_j \tag{9}$$

being C_{ij} the elastic constants, e_i the strain components and V the volume of the material. In the case of a bulk deformation, this equation leads to

$$\frac{E_{elastic,bulk}}{V} = \frac{9\varepsilon^2}{2} K \tag{10}$$

where $K = \frac{1}{3}\left(C_{11} + 2C_{12}\right)$ is the bulk modulus. Comparing the previous equation with equation (7) it is obtained that

$$K = \frac{1}{18V}\sum\sum_{k\neq k'} \left(r^0_{kk'}\right)^2 U''\left(r^0_{kk'}\right). \tag{11}$$

This latter double sum can be written as N_{at} (that is the total number of atoms in the material) multiplied by the mean value of a single sum taken with respect to one central atom, that is

$$K = \frac{1}{18V_{at}}\left\langle \sum r_k^2 U''\left(r_k\right)\right\rangle \tag{12}$$

where now r_k is the distance from the central atom towards a neighbouring atom k in the undeformed situation, and $V_{at} = V/N_{at}$ is the mean atomic volume.

In the case of a uniform shear deformation the position of an atom k can be written as

$$\mathbf{r}_k = \mathbf{r}^0_k - \alpha x^0_k \mathbf{e}_x + \alpha y^0_k \mathbf{e}_y \tag{13}$$

where x^0_k, y^0_k are the coordinates of the undeformed atomic position, $\mathbf{e}_x$, $\mathbf{e}_y$ are the unitary vectors on the x and y directions and α is a small number describing the deformation. Substituting the above expression in equation (5) and by means of a Taylor expansion upto second order in α, it is obtained that

$$E_{elastic,shear} = \frac{\alpha^2}{6}\sum\sum_{k\neq k'} \left(r^0_{kk'}\right)^2 U''\left(r^0_{kk'}\right) - \frac{3\alpha^2}{2}\sum\sum_{k\neq k'} \left(x^0_{kk'}\right)^2 \left(y^0_{kk'}\right)^2 \left(\frac{U''\left(r^0_{kk'}\right)}{\left(r^0_{kk'}\right)^2} - \frac{U'\left(r^0_{kk'}\right)}{\left(r^0_{kk'}\right)^3}\right) \tag{14}$$

where $x^0_{kk'}$ is the x coordinate of $\mathbf{r}^0_k - \mathbf{r}^0_{k'}$ and so on. Using the general expression of the elastic energy in a stressed material of equation (9), and introducing a deformation field as

the one defined by α in equation (13) it is obtained that

$$\frac{E_{elastic,shear}}{V} = 2\alpha^2 G \tag{15}$$

where $G = \frac{1}{2}(C_{11} - C_{12})$ is the shear modulus. Combining the two previous equations, and following an identical procedure as for the bulk modulus, the shear modulus in terms of the mean value of the sum over the neighbours of a central atom is written as

$$G = \frac{1}{12V_{at}}\left[\left\langle \sum r_k^2 U''(r_k)\right\rangle - 9\left\langle \sum x_k^2 y_k^2 \left(\frac{U''(r_k)}{r_k^2} - \frac{U'(r_k)}{r_k^3}\right)\right\rangle\right]. \tag{16}$$

Likewise in equation (12), x_k, y_k and r_k now correspond to the position of the neighbouring atoms respect to the central atom in the undeformed situation. After some manipulation profiting from the isotropy in amorphous materials, the last expression becomes

$$G = \frac{1}{30V_{at}}\left[\left\langle \sum r_k^2 U''(r_k)\right\rangle + \frac{3}{2}\left\langle \sum r_k U'(r_k)\right\rangle\right]. \tag{17}$$

Details of the mathematical derivation are found in ref.[11].

Finally, using the bulk and shear moduli expressions given in equations (12) and (17) their ratio becomes

$$\frac{K}{G} = \frac{5}{3}\left[1 + \frac{3}{2}\frac{\langle \sum r_k U'(r_k)\rangle}{\langle \sum r_k^2 U''(r_k)\rangle}\right]^{-1}, \tag{18}$$

where $K/G = 5/3$, or equivalently $\nu = 0.25$, correspond to the Cauchy relation for an ideal isotropic solid with the absence of defects and anharmonicity.

The expressions of K and G given above are the so-called "Born terms" and they assume strictly uniform deformations. However, in amorphous solids the elastic moduli have the contribution of elastic relaxations, that is the atomic rearrangements leading to local states of lower energy during a global deformation. In metallic glasses, molecular dynamic simulations show that elastic relaxations lower K and G about a 10% and more than a 30% of the respective uniform deformation values[13][14]. The Knuyt model used in the present work allows the estimation of the rearrangement terms of K and G[11]. However, their inclusion would not change qualitatively the results that will be presented in section 3. As we are interested here in describing qualitatively the effect of the structural changes on the Poisson's ratio and for the sake of simplicity we will not take into account these rearrangement terms. Further discussion on what would be the effect of including these terms will be given in section 3.

Now, the elastic moduli expressions described above can be calculated using the RDF of equation (3). The averages in equations (12) and (17) are calculated as

$$\begin{array}{c} \left\langle \sum r_k^2 U''\left(r_k\right)\right\rangle = \int_{r=0}^{\infty} r^2 U''\left(r\right) RDF\left(r\right) dr \\ \left\langle \sum r_k U'\left(r_k\right)\right\rangle = \int_{r=0}^{\infty} r U'\left(r\right) RDF\left(r\right) dr \end{array}, \tag{19}$$

that is substituting the sums over the neighbouring atoms by the mean value calculated using the proposed RDF. Therefore, the elastic moduli K and G are obtained in terms of the parameters determining the RDF (r_1 and σ_1) and the parameters determining the interatomic potential (r_m, a and b). Defining δ as the distance between the mean position of the first shell of neighbours in the RDF and the position of the interatomic potential minimum

$$r_1 = r_m + \delta, \tag{20}$$

the result obtained for the elastic moduli K and G from equations (12), (17) and (19) can be conveniently expressed in terms of three non-dimensional parameters

$$s = \tfrac{\delta}{r_m},\ \sigma = \tfrac{\sigma_1}{r_m},\ p = \tfrac{br_m}{a}\,. \tag{21}$$

Parameters s and σ account respectively for the mean atomic position displacement from r_m and the mean atomic dispersion around such value. Parameter p, which is negative, gives a measure of the anharmonicity of the potential. Indeed, the position of the inflection point after the minimum of the potential of equation (4) is given by $r_m\left(1-\frac{1}{3p}\right)$. The result obtained for K and G cutting off the high order terms in s and σ is given by

$$K = \frac{aN_1 r_m^2}{9V_{at}}\left[1 + 3s\left(1+p\right) + 3s^2\left(1+3p\right) + 3\sigma^2\left(1+3p\right) + ...\right], \tag{22}$$

and

$$G = \frac{aN_1 r_m^2}{15V_{at}}\left[1 + \frac{3}{2}s\left(3+2p\right) + \frac{3}{4}s^2\left(8+15p\right) + \frac{3}{4}\sigma^2\left(8+15p\right) + ...\right]. \tag{23}$$

These simplified expressions allow a quick examination of the K and G dependencies on s and σ. Nevertheless, the integrations in equation (19) can be evaluated without cutting off the higher order terms. The results presented in the next section were obtained using the complete result of the integration.

III. RESULTS AND DISCUSSION

In order to evaluate the behaviour of K and G it is needed to give some value for p, in this work $p = -1.747$ is chosen. This value correponds to an interatomic potential for Iron with $a = 0.957\text{eV}\text{Å}^{-2}$, $b = -0.639\text{eV}\text{Å}^{-3}$ and $r_m = 2.617\text{Å}$ used in classical defect simulations[15]. From literature data it is found that values of p from -1.5 to -2.5 are realistic for most metals. Actually, the results presented in this section do not vary qualitatively for any value of p within this range. Figures 1 and 2 show the variation of K, G and K/G when varying parameter s and σ. In such plots the bulk and shear moduli are normalized by $K_0 = \frac{aN_1 r_m^2}{9V_{at}}$ and $G_0 = \frac{aN_1 r_m^2}{15V_{at}}$. The calculations are performed using a constant $\sigma = 0.063$ for figure 1 and a constant $s = -0.018$ for figure 2, these values correspond to realistic values of $\sigma_1 = 0.165\text{Å}$ and $r_1 = 2.57\text{Å}$ obtained in experimental diffraction data for the first Fe-Fe peak in $Fe_{80}B_{20}$ amorphous alloys[16]. Nevertheless, the elastic constants behaviour depicted in figures 1 and 2 does not present remarkable differences when using any σ or s values within a realistic range.

Figures 1 and 2 show the increase in the elastic constants K and G when decreasing either s or σ. The same behaviour would be obtained for the Young modulus $E = 9K/\left(3K/G + 1\right)$. This is in agreement with the experimental observation of increase of the elastic moduli E, G and K of metallic glasses after structural relaxation and under increasing pressure[1][2][3][4][5]. In the case of metals and especially transition-metals, the short-range ionic interactions - which are well-described by a central potential like the one used in the present approach - are expected to be the main contribution to the elastic constants. Therefore, the reduction of the interatomic distances, when either T_f decreases or pressure increases, is expected to enhance the elastic stiffness of the glass. Here it is worth to recall that this behaviour is not general for other chemically distinct glasses. As an example, the increase in pressure reduces the elastic moduli in many oxide glasses as in the case of window glass[17].

In the case of K/G or equivalently the Poisson's ratio ν, the results obtained from the model show an opposite dependence on s and σ. Poisson's ratio increases as s decreases, but it is found to reduce its value as σ decreases. Both σ and s are expected to become smaller due to the increase of ρ in structural relaxation and when increasing hydrostatic pressure. However, it is well-known that the structural change during glass relaxation, or equivalently

when reducing temperature in an equilibrium liquid, is mainly concerned with the reduction of the dispersion in the RDF peaks. On the other hand, high-pressure treatments of already formed metallic glasses are expected to reduce s and σ in a reversible way, that is elastically deforming the structure but without atomic rearrangements leading to a higher short-range order. Up to 0.5GPa there is not observed any density change of metallic glasses once released after the pressure test[4].

Hence, the results shown in figures 1 and 2 may explain qualitatively the experimental observations of the K/G ratio decrease when reducing T_f and increase when increasing pressure. In the first case, the reduction of σ would have a dominant effect on the structural change of the glass thus reducing K/G. In the latter case, the reduction in s would be dominant thus resulting in an increase of the K/G ratio. Indeed, supposing a proportional reduction of s and σ^2 given by $\Delta s = C\Delta\sigma^2$ with $C =$*constant*, as may be expected in a reduction of the mean atomic volume, the value of C determines the behaviour of K/G. The slope $\frac{d(K/G)}{d\rho} \propto -\frac{d(K/G)}{ds}$ changes from negative values (the decrease in σ is dominant) to postive values (the decrease in s is dominant) at a certain value of C. As an example, in the case of $\sigma_1 = 0.165$Å and $r_1 = 2.57$Å used in the previous calculations such change in the K/G behaviour is found at a value of $C = 0.755$.

It is interesting to remark that, as shown from equations (23) and (22), although the values of K and G are directly dependent on the first-shell coordination number N_1, the K/G ratio is not affected by any change in N_1. This means that when reducing the T_f of a glass the predicted reduction of ν is due mainly to the change in σ but not to the change in the coordination number of the first RDF peak. Similarly, the interatomic force constant a does affect K and G values while K/G is just affected by the shape (or equivalently the anharmonicity) of the potential, which in this model is determined by the parameter p.

As already discussed, equations (23) and (22) does not take into account the influence of the elastic relaxation. Contrary to the main structural relaxation due to aging, elastic relaxations are fast, with times of the order of picoseconds, and so their contribution should be taken into account when considering experimental ultrasonic measurements of the elastic properties. However, the inclusion of the rearrangement terms given by the Knuyt model does not change the tendencies of K, G and K/G shown in figures 1 and 2. Firstly, the rearrangement terms does not have a first order contribution of the parameter s, and then no significant changes are expected on the behaviour of K, G and K/G shown in figure 1.

Secondly, the rearrangement terms dependence on σ^2 shows a greater influence on G than on K. Although the absolute values of both G and K are reduced when considering the rearrangement terms, the effect of these terms is a proportional bigger increase of G than K when decreasing σ, this leading to a bigger decrease of K/G than the one shown in figure 2. A first order approximation expressions of the K and G rearrangement terms are given in ref.[11]. Therefore, the qualitative description of the general tendencies of the elastic moduli observed experimentally in metallic glasses under structural changes is mainly associated to the behaviour of the Born terms of K and G, which would correspond to the instantaneous K and G moduli measured in an ideally infinite frequency experiments.

From experimental data, the fragility of a super-cooled liquid was found to be correlated with the K/G ratio for a wide set of chemically-different glasses[7]. Stronger glasses were found to have lower values of K/G. Examining the existing data for metallic glasses in the literature, it seems that such correlation is not maintained when looking at alloys with similar values of K/G, although a roughly correlation still exists when looking at a wide set of alloy compositions. A strong liquid-alloy is expected to have more short-range order in the super-cooled region than a fragile one, so inhibiting atomic rearrangements and increasing viscosity. The viscosity behaviour in the super-cooled region have to be dependent on many structural details of the liquid, as well as on the particular characteristics of the interatomic forces between atoms or molecules. A proper assessment of a fragility-elastic constants relationship can not be realised by the simple model presented here. Notwithstanding, from the results presented here, in the case of similar values of the interatomic forces, a stronger liquid, which is then expected to have a lower value of σ, would have lower instantaneous K/G ratio.

As already discussed, the model originally developed by Knuyt et al., which uses a very simple structural model of a metallic glass, describes qualitatively the changes of the elastic constants observed in structural relaxation and in hydrostatic pressure tests. However, great precautions have to be taken into account when using these results to explain the behaviour of metallic glasses. First of all, the model account for an ideal uni-component metallic glass, while all available experimental results refer to multi-component metallic glasses. Moreover, the central interatomic potential used in the model seems a reasonable approach just for transition metals, where the electronic contribution to the elastic constants is known to be small and directional bonding is expected to have a very low influence. Indeed,

it seems reasonable that no qualitative changes have to be expected if the Iron potential used in this work was changed by a potential corresponding to any other transition metal. However, most metallic glass compositions have non-transition metals and metalloids as main components. Finally, the approach realized does not take into account any influence on the elastic properties of the second and third coordination shells. In a more complex atomic structure made-up with atoms of different sizes densely packed the contributions of the second and third shells are likely to be important.

These and other limitations of the model suggest that important changes in the predicted elastic constants behaviour may be found if we were able to introduce a more detailed knowledge of the atomic structure and the interatomic forces. On the other hand, the simplicity of the model, with just two parameters determining the structure of the glass, offers a very intuitive idea of the way structural changes affect the elastic constants in metallic glasses. Molecular dynamic simulations would be the ideal tool to check if similar behaviours are obtained for a more complex model of a glass.

IV. CONCLUSIONS

A model developed by Knuyt et al. (1990 and 1991) was used to explain qualitatively the Poisson's ratio behaviour during structural changes in metallic glasses. The reduction of the mean atomic volume leads to a reduction of both the position (r_1) and the width (σ_1) of the first peak of the radial atomic distribution function of an amorphous metal. The model shows that the change of the Poisson's ratio is opposite when decreasing r_1 or σ_1. This may explain the experimentally found opposite behaviour of the Poisson's ratio in glass relaxation and in hydrostatic pressure tests. However, in order to assess the correctness of the model predictions and get quantitative results for actual glass-forming alloys, a more complex structural model than the one presented here would be necessary.

Many mechanical properties of metallic glasses seem to be critically related to the value of the elastic constants. Although technologically complex, the results presented in this work suggest that the application of pressure treatments during metallic glass vitrification could result in glasses with interesting different mechanical properties.

Acknowledgments

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FIG. 1: Bulk (K) and Shear (G) moduli and the ratio G/K as a function of the mean atomic position s of the first neighbours shell

FIG. 2: Bulk (K) and Shear (G) moduli and the ratio G/K as a function of the atomic dispersion σ of the first neighbours shell

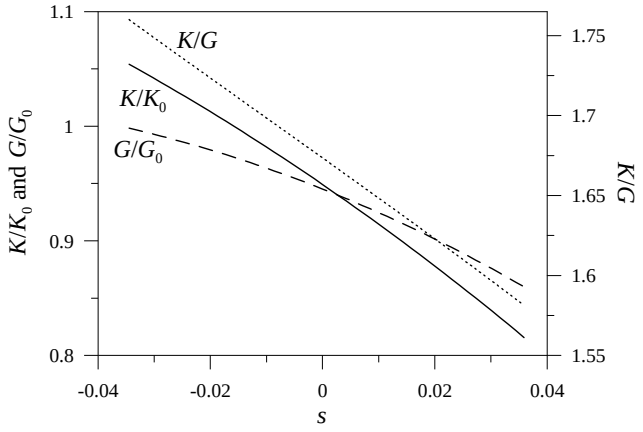

Figure 1.

Figure 1

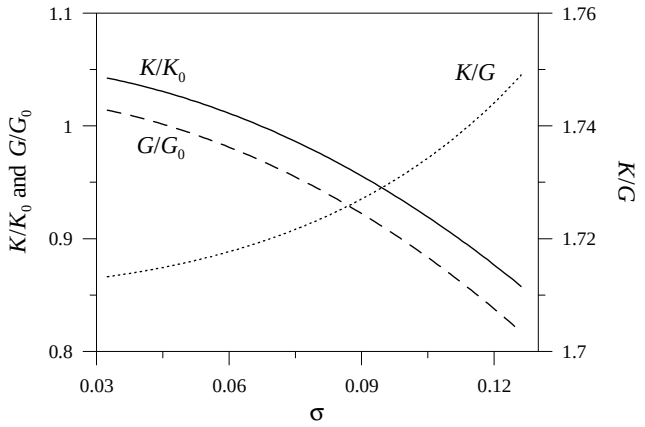

Figure 2.

Figure 2