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Continuum theory of internal stresses in amorphous metals

R Pawellek and M Fähnle

Institut für Physik, Max-Planck-Institut für Metallforschung, Heisenbergstrasse 1, 7000 Stuttgart 80, Federal Republic of Germany

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Abstract. Within the framework of the local linearised theory of elasticity, internal stresses in amorphous metals have been calculated using a Green function perturbation approach based on the incompatibility method. A simple model is introduced to describe the development of structural incompatibilities during the quenching process of the liquid metal, which are the sources for the internal stresses. The results are compared with those for the atomic-level stresses obtained with computer simulation studies by Egami and co-workers, and with the results derived by these authors from a continuum theory based on Eshelby's inclusion problem.

1. Introduction

Whereas a perfect crystal is stress-free, deviations from the ideal lattice represent sources for internal stresses, i.e. stresses which can exist without the action of external forces (self-stresses; cf Kröner 1974). Examples are vacancies and interstitials, which exist in any crystal at non-zero temperature, or dislocations produced by non-equilibrium processes such as crystallisation and plastic deformation. In an amorphous material there are stresses at the atomic level because of the lack of atomic order. These atomic-level stresses are defined at any atomic position and result from the incompatibility between a given atom and its environment. They have been defined on a quantum-mechanical basis by Vitek and Egami (1987) and have been used by Egami and co-workers (see, e.g., Egami *et al* 1980, Srolovitz *et al* 1981a, b) to characterise the local topology and symmetry of a computer-generated amorphous structure.

To illuminate the physical meaning of the local structural incompatibilities producing atomic-level stresses it is very instructive (Vitek and Egami 1987, Egami and Srolovitz 1982) to extend the continuum elasticity theory to the atomic scale. An especially illuminating approach was the application of Eshelby's (1957) theory of spherical inclusions in an elastic medium, identifying the inclusion with an atom which in an amorphous structure does not ideally fit into the environment as would be the case in a perfect crystal. Thereby the spherical inclusion is a special example for a structural incompatibility. It is therefore tempting to characterise the amorphous structure in a reasonable way by a field of incompatibilities. To do this we can in principle start from a topological model of the amorphous structure, for instance that of Kléman and Sadoc (1979), as discussed in the paper by Vitek and Egami (1987). In the present paper

we calculate the incompatibilities approximately from a simple model describing the distribution of thermal strains in the thermal equilibrium of the liquid material before the amorphous structure is obtained by quenching.

Having defined the incompatibilities, the internal stresses may be calculated by the so called incompatibility method of elasticity theory, which was introduced by Reissner (1931) and developed further by Kröner (1958) for his theory of dislocations in crystals. It is well known that continuum theories can be extended to the atomic scale, but that in this case in principle a non-local theory should be applied because of the discreteness of the structure and the finite range of interactions between the atoms (Kröner 1967). However, it was also conjectured (Vitek and Egami 1987) that a local approximation suffices for general, qualitative considerations for which no very precise numbers are demanded. In the present paper we therefore confine ourselves to the local linearised theory of elasticity.

The present approach, that is modelling of the incompatibilities and solution of the elastic problem by the incompatibility method, has already been applied successfully to the calculation of the effective magnetostriction tensor of amorphous and polycrystalline ferromagnets (Furthmüller *et al* 1986, 1987a, b, Pawellek *et al* 1988, Fähnle *et al* 1988a, b). In this case the incompatibilities arise from the various spontaneous magnetostrictive strains that the differently oriented structural units would exhibit if they were elastically decoupled. In the present case the incompatibilities arise from the different thermal expansions that the isolated volume elements would exhibit in the melt as a result of thermal fluctuations. In both cases the structural units are described on a phenomenological level by introducing local material tensors, for example the local tensor of the elastic constants or the local magnetostriction tensor, instead of taking into account the detailed atomic structure.

From the incompatibilities we calculate the total strains $\varepsilon_{ij}(\mathbf{r})$ and the stresses $\sigma_{ij}(\mathbf{r})$ by the incompatibility method. Thereby we are not interested in the detailed knowledge of the position dependence of ε_{ij} and σ_{ij} , but in correlation functions of the type $\langle \varepsilon_{ij}(\mathbf{r}) \rangle$, $\langle \varepsilon_{ij}(\mathbf{r}) \varepsilon_{kl}(\mathbf{r}') \rangle$, $\langle \sigma_{ij}(\mathbf{r}) \rangle$ and $\langle \sigma_{ij}(\mathbf{r}) \sigma_{kl}(\mathbf{r}') \rangle$. To calculate them we must introduce some statistical assumptions (§ 2). Volume and ensemble averages will be regarded as identical, that is we consider an ergodic situation.

For the stresses, the average value $\langle \sigma_{ij}(\mathbf{r}) \rangle$ is zero due to the theorem of Albenga (1918 + 1919). Therefore we will concentrate on the tensor of the correlation functions $\langle \sigma_{ij}(\mathbf{r}) \sigma_{kl}(\mathbf{r}') \rangle$ for $\mathbf{r} = \mathbf{r}'$ for the two invariant combinations of its components respectively, the hydrostatic pressure $\sqrt{\langle p^2 \rangle}$ and von Mises' (1913) shear stress $\sqrt{\langle \tau^2 \rangle}$, with

$$p^2 = \left(\frac{1}{3} \text{Tr } \boldsymbol{\sigma} \right)^2 = \frac{1}{9} \sigma_{ii} \sigma_{jj} \quad (1)$$

$$\tau^2 = \frac{1}{2} \sigma_{ij} \sigma_{ji} - \frac{1}{6} \sigma_{ii} \sigma_{jj}. \quad (2)$$

In equations (1) and (2) and in the following we adopt Einstein's summation convention.

For the strains, both the average value $\langle \varepsilon_{ij}(\mathbf{r}) \rangle$ as well as the correlation functions $\langle \varepsilon_{ij}(\mathbf{r}) \varepsilon_{kl}(\mathbf{r}') \rangle$ are of interest. We can define in an analogous way invariant measures for the length dilatation $\sqrt{\langle l^2 \rangle}$ (which is $\frac{1}{3}$ of the volume dilatation) and von Mises' shear strains $\sqrt{\langle s^2 \rangle}$ (which vanish for isotropic strain $\varepsilon_{ij} = \lambda \delta_{ij}$) by

$$l^2 = \frac{1}{9} \varepsilon_{ii} \varepsilon_{jj} \quad (3)$$

$$s^2 = \frac{1}{2} \varepsilon_{ij} \varepsilon_{ji} - \frac{1}{6} \varepsilon_{ii} \varepsilon_{jj}. \quad (4)$$

Our paper is organised as follows. In § 2 we introduce the general formalism of the

incompatibility method which allows us to calculate the internal stresses from the incompatibilities. This formalism is the same as that used for the calculation of the effective magnetostriction tensor from the magnetostrictive incompatibilities of an amorphous material (Furthmüller *et al* 1986, 1987a, b, Pawellek *et al* 1988, Fähnle *et al* 1988a, b). In § 3 we will discuss our simple model for the calculation of the structural incompatibilities in amorphous metals. The results of the calculations for the strains and internal stresses are given in § 4, where we also compare our approach in detail with the continuum theory of Egami and Srolovitz (1982) based on Eshelby's (1957) inclusion problem.

2. The incompatibility method

To illustrate the basic concept of the method the following gedanken experiment is performed. First we define the state of the system without the incompatibilities under consideration as the reference state. For the calculation of the effective magnetostriction tensor of amorphous ferromagnets, this state is the amorphous state with the exchange interactions between the magnetic moments switched off, i.e. without magnetisation and without magnetostrictive deformations. It should be noted that due to the atomic-level stresses this state is not stress-free for an amorphous system. For the calculation of the atomic-level stresses we consider in the present paper the perfectly ordered crystalline state as the reference state.

We now cut the system into very small structural units. For both calculations those units consist basically of an atom and its nearest-neighbour atoms. In the magnetostriction case this is motivated by the fact that the local magnetic anisotropy, which is responsible for magnetostriction in amorphous ferromagnets, varies randomly from site to site (Elsässer *et al* 1988). For the calculation of atomic-level stresses we introduce the incompatibilities by considering the different thermal expansions that the volume elements would exhibit in the melt (§ 3). It is reasonable to assume that in the melt clusters of an atom and its nearest-neighbour atoms may be considered to be more or less independent. It should be noted that in the case of the amorphous reference state for the magnetostriction problem we do not allow for relaxation processes during the cutting procedure which would remove the atomic-level stresses. We can therefore at this stage of the gedanken experiment again weld together the volume elements to a compact material.

In the next step of the gedanken experiment we allow for so called quasiplastic deformations of the volume elements. In the magnetostriction case the quasiplastic deformations are introduced by switching on the exchange interactions and applying a very strong external magnetic field, so that all units have a magnetisation in the same direction. As a result the units will exhibit spontaneous magnetostrictive strains like small monocrystalline ferromagnets, and because of the random orientations of the magnetic anisotropy axes all the units are deformed in a different way. Because the structural units retain this state of spontaneous magnetostrictive deformation without support of external forces (as in the case of plastic deformation of a crystal), the magnetostrictive strains $\epsilon_{ij}^{\text{mag}}$ belong to the class of quasiplastic deformations ϵ_{ij}^{Q} , which are by definition stress-free. For the calculation of atomic-level stresses in amorphous metals we associate the quasiplastic deformations with the thermal expansions that the isolated units will experience when exposed to a heat bath. The coupling to a heat bath thereby simulates the situation of the system before quenching it to the amorphous state.

These quasiplastic deformations are also different for different units because of the thermal fluctuations (§ 3), and they are frozen by the quenching process.

After the introduction of the spatially fluctuating quasiplastic deformations ε_{ij}^Q the units no longer fit together to a compact material. Additional elastic strains $\varepsilon_{ij}^{el}(\mathbf{r})$ are required to restore compatibility of the material in the last step of the gedanken experiment, and the total strain $\varepsilon_{ij}(\mathbf{r})$ is given by

$$\varepsilon_{ij}(\mathbf{r}) = \varepsilon_{ij}^Q(\mathbf{r}) + \varepsilon_{ij}^{el}(\mathbf{r}). \quad (5)$$

For given quasiplastic strains $\varepsilon_{ij}^Q(\mathbf{r})$ the elastic strains $\varepsilon_{ij}^{el}(\mathbf{r})$ therefore must be determined in such a way that

$$\text{Ink}(\boldsymbol{\varepsilon}^Q(\mathbf{r}) + \boldsymbol{\varepsilon}^{el}(\mathbf{r})) = 0. \quad (6)$$

Furthermore, the balance-of-force equation must be fulfilled, which in the absence of external forces is given by

$$\text{Div } \boldsymbol{\sigma} = 0. \quad (7)$$

$\boldsymbol{\sigma}$ denotes the tensor of elastic stresses, which are related to the elastic strains by

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl}^{el} \quad (8)$$

where C_{ijkl} denotes the tensor of the elastic constants.

Equations (6)–(8) may be formally solved using the (yet unknown) stress Green tensor $\Delta_{ijkl}(\mathbf{r}, \mathbf{r}')$ via

$$\sigma_{ij}(\mathbf{r}) = \int d^3 r' \Delta_{ijkl}(\mathbf{r}, \mathbf{r}') \varepsilon_{kl}^Q(\mathbf{r}'). \quad (9)$$

In the case of an infinitely extended homogeneous isotropic medium, Δ_{ijkl} can be calculated explicitly (Kröner and Koch 1976, Kröner 1986) and is given in k -space by

$$\Delta_{ijkl}^{(0)}(\mathbf{k}) = -C_{ijkl}^{(0)} - C_{ijmn} \Gamma_{(mn)(pq)}^{(0)}(\mathbf{k}) C_{pqkl}^{(0)} \quad (10)$$

with

$$\Gamma_{ijkl}^{(0)}(\mathbf{k}) = [(3K_0 + G_0)/G_0(3K_0 + 4G_0)](k_i k_j k_k k_l / k^4) - (1/G_0)(k_i k_k \delta_{jl} / k^2). \quad (11)$$

Here $C_{ijkl}^{(0)}$, K_0 and G_0 denote the tensor of the elastic constants, the bulk modulus and the shear modulus of the homogeneous isotropic medium.

In the amorphous material the tensor of the elastic constants is a spatially fluctuating quantity. To model the situation in a phenomenological frame it has been assumed (Furthmüller *et al* 1986, 1987a, b, Pawellek *et al* 1988, Fähnle *et al* 1988a, b) that the small structural units are all identical in their own reference frame and exhibit well defined anisotropy. Due to the random orientation of the anisotropy axes the tensor of the elastic constants $C_{ijkl}(\mathbf{r})$ and the tensor of the elastic compliances $S_{ijkl}(\mathbf{r})$ in an external fixed coordinate system exhibit spatially random fluctuations, and the volume average $\langle C_{ijkl}(\mathbf{r}) \rangle$ yields an isotropic tensor.

For spatially fluctuating material parameters the stress Green tensor $\Delta_{ijkl}(\mathbf{r}, \mathbf{r}')$ cannot be calculated explicitly. In this case the stress $\sigma_{ij}(\mathbf{r})$ may be calculated by a Green function perturbation theory with the fluctuations $\delta S_{ijkl}(\mathbf{r}) = S_{ijkl}(\mathbf{r}) - \langle S_{ijkl}(\mathbf{r}) \rangle$ as perturbation parameter (Kröner and Koch 1976, Kröner 1986, Furthmüller *et al* 1987a, Fähnle *et al* 1988b). In the following we restrict our considerations to the zeroth-order

perturbation, i.e. we neglect all terms containing the fluctuation δS_{ijkl} , yielding

$$\sigma_{ij}(\mathbf{r}) = \int d^3r' \Delta_{ijkl}^{(0)}(\mathbf{r} - \mathbf{r}') \varepsilon_{kl}^Q(\mathbf{r}') \quad (12)$$

where $\Delta_{ijkl}^{(0)}$ denotes the Green stress tensor for a hypothetical homogeneous isotropic medium with the tensor $\langle C_{ijkl}(\mathbf{r}) \rangle$ of elastic constants. If the structural units of our amorphous material had isotropic elastic properties, the zeroth-order term would yield the exact solution.

From equation (12) we obtain

$$\langle \sigma_{ij}(\mathbf{r}) \sigma_{kl}(\mathbf{r}') \rangle = \int d^3r'' d^3r''' \Delta_{ijmn}^{(0)}(\mathbf{r} - \mathbf{r}'') \Delta_{klpq}^{(0)}(\mathbf{r}' - \mathbf{r}''') \langle \varepsilon_{mn}^Q(\mathbf{r}'') \varepsilon_{pq}^Q(\mathbf{r}''') \rangle. \quad (13)$$

To evaluate these correlation functions we need as statistical input the correlation functions $\langle \varepsilon_{mn}^Q(\mathbf{r}'') \varepsilon_{pq}^Q(\mathbf{r}''') \rangle$ of the quasiplastic strains. In the following we assume that the quantities may be written as

$$\langle \varepsilon_{mn}^Q(\mathbf{r}'') \varepsilon_{pq}^Q(\mathbf{r}''') \rangle = \langle \varepsilon_{mn}^Q(\mathbf{r}'') \rangle \langle \varepsilon_{pq}^Q(\mathbf{r}''') \rangle + g(\mathbf{r}'' - \mathbf{r}''') \langle \delta \varepsilon_{mn}^Q(\mathbf{r}'') \delta \varepsilon_{pq}^Q(\mathbf{r}''') \rangle \quad (14)$$

with $\delta \varepsilon_{mn}^Q = \varepsilon_{mn}^Q - \langle \varepsilon_{mn}^Q \rangle$. The averages $\langle \varepsilon_{mn}^Q \rangle$ and $\langle \delta \varepsilon_{mn}^Q(\mathbf{r}) \delta \varepsilon_{pq}^Q(\mathbf{r}') \rangle$ are determined by a simple model calculation in the next section. Furthermore, taking into account the properties of the stress Green tensor $\Delta_{ijkl}^{(0)}$, it may be shown that for $\mathbf{r} = \mathbf{r}'$, that is for the calculation of $\langle \sigma_{ij}(\mathbf{r}) \sigma_{kl}(\mathbf{r}) \rangle$ for example, we do not need the explicit form of the function $g(\mathbf{r}'' - \mathbf{r}''')$ of equation (14) but just the properties $g(0) = 1$ and $g(\infty) = 0$. We then can solve the integrals in equation (13) analytically in k -space, yielding

$$\langle \sigma_{ij}(\mathbf{r}) \sigma_{kl}(\mathbf{r}) \rangle = T_{ijmnlkpq} \langle \delta \varepsilon_{mn}^Q(\mathbf{r}) \delta \varepsilon_{pq}^Q(\mathbf{r}) \rangle \quad (15)$$

where the tensor T is composed of combinations of the material parameters K_0 and G_0 . From equation (15) we then can calculate the hydrostatic pressure and von Mises' shear stress according to equations (1) and (2). The total strain $\varepsilon_{ij}(\mathbf{r})$ is given by

$$\varepsilon_{ij}(\mathbf{r}) = \varepsilon_{ij}^Q(\mathbf{r}) + \varepsilon_{ij}^{el}(\mathbf{r}) = \varepsilon_{ij}^Q + S_{ijkl} \sigma_{kl}. \quad (16)$$

In the zeroth-order approximation ($\delta S_{ijkl} = 0$) this yields

$$\langle \varepsilon_{ij}(\mathbf{r}) \rangle = \langle \varepsilon_{ij}^Q \rangle + S_{ijkl} \langle \sigma_{kl} \rangle = \langle \varepsilon_{ij}^Q \rangle \quad (17)$$

where we have used the theorem of Albenga (1918 + 1919). This means that the volume average of the total strain is in the zeroth-order approximation exclusively determined by the quasiplastic strains, whereas the elastic part averages out. From equations (15) and (16) we can calculate the quantities $\langle \varepsilon_{ij}(\mathbf{r}) \varepsilon_{kl}(\mathbf{r}) \rangle$ and then according to equations (3) and (4) the invariants l and s . Of course, for these quantities as well as for the whole distribution function for $\varepsilon_{ij}(\mathbf{r})$, the elastic part ε_{ij}^{el} will also play a role.

3. Model for the quasiplastic strains

In this section we discuss a simple model to introduce into the system the quasiplastic strains responsible for the atomic-level stresses in amorphous materials. The starting point is the fact that the amorphous state is obtained in the experimental quenching procedure, i.e. by freezing the liquid-like structure of the system. To a rough approximation the liquid may be modelled by considering small structural units, consisting

basically of an atom and the nearest-neighbour atoms. The units are swimming in a heat bath with characteristic temperature T^c , which may be identified with the temperature just before the freezing in the quenching process takes place, probably a temperature between the melting temperature and the glass temperature. In the heat bath the units are thermally expanded compared with their state at low temperature. Because a thermal strain is maintained without the support of any external forces, it belongs to the class of quasiplastic strains ϵ_{ij}^Q . As a result of the thermal fluctuations in the heat bath, there is a distribution of quasiplastic strains with a probability density function $p(\epsilon^Q)$ given by a Boltzmann distribution

$$p(\epsilon^Q) \sim \exp[-W(\epsilon^Q)/kT]. \quad (18)$$

Here $W(\epsilon^Q)$ is the increase of energy of the unit associated with the thermal expansion. For $W(\epsilon^Q)$ we consider two different ansatzes.

(i) The energy $W(\epsilon^Q)$ depends only on the volume dilatation $\Delta V/V = \text{Tr } \epsilon^Q$ and can be expanded as

$$W(\epsilon^Q) = V_0[(1/2!)C^{(2)}(\text{Tr } \epsilon^Q)^2 + (1/3!)C^{(3)}(\text{Tr } \epsilon^Q)^3 + (1/4!)C^{(4)}(\text{Tr } \epsilon^Q)^4 + \dots]. \quad (19)$$

In this case the volume elements may be called liquid because their energy does not depend on the shear strains. The quantity V_0 denotes the volume of the structural unit and is the only microscopic quantity which enters our theory. The quantity $C^{(2)}$ is the bulk modulus of the structural unit.

(ii) The energy $W(\epsilon^Q)$ depends on all components of ϵ^Q , i.e.

$$W(\epsilon^Q) = V_0[(1/2!)C_{ijkl}\epsilon_{ij}^Q\epsilon_{kl}^Q + (1/3!)C_{ijklmn}\epsilon_{ij}^Q\epsilon_{kl}^Q\epsilon_{mn}^Q + (1/4!)C_{ijklmnpq}\epsilon_{ij}^Q\epsilon_{kl}^Q\epsilon_{mn}^Q\epsilon_{pq}^Q + \dots]. \quad (20)$$

In this case the volume elements may be regarded as solid.

The quantities of interest, $\langle \epsilon_{ij}^Q(\mathbf{r}) \rangle$ and $\langle \epsilon_{ij}^Q(\mathbf{r})\epsilon_{kl}^Q(\mathbf{r}) \rangle$, entering equations (13) and (14) may be calculated analytically from equations (18)–(20) when confining to the quadratic terms in equations (19) and (20). The price we have to pay is that in this linear approximation the volume average $\langle \epsilon_{ij}^Q \rangle$ vanishes, and hence, according to equation (17), there is no macroscopic deformation $\langle \epsilon_{ij} \rangle$ due to the internal structural incompatibilities. This is in contrast to the experimental fact that the specific volume of the amorphous system is larger than that of the corresponding crystalline system. The difference, which is of the order of a few per cent, is called the free volume (see, e.g., Kronmüller 1981, 1984, Brandt and Kronmüller 1983). Indeed, when going beyond the linear approximation by numerical calculation and when inserting reasonable values for the higher-order coefficients $C^{(3)}$ and $C^{(4)}$, we obtain from equation (19) a free-volume effect of the right order of magnitude. Because the inclusion of the higher-order terms of equations (19) and (20) yields only a relatively small modification of the quantities $\langle \epsilon_{ij}^Q(\mathbf{r})\epsilon_{kl}^Q(\mathbf{r}) \rangle$, we confine ourselves to the quadratic terms in the energy expressions. In case (i) this yields

$$\langle \delta \epsilon_{ij}^Q \delta \epsilon_{kl}^Q \rangle = (1/9)(kT/C^{(2)}V_0)\delta_{ij}\delta_{kl}. \quad (21)$$

For case (ii) we consider a cubic anisotropy of the volume elements which is reasonable for the case of iron for which we present the results in § 4. Because the volume elements are randomly distributed in the melt with respect to their orientation, the ensemble

average (symbol $\langle \rangle$) includes an average over all orientations. Altogether, we obtain

$$\langle \delta \varepsilon_{11}^0 \delta \varepsilon_{11}^0 \rangle = \frac{1}{6} [(3C_{11} + C_{12}) / (C_{11} - C_{12})(C_{11} + 2C_{12}) + 1/C_{44}] kT/V_0 \quad (22)$$

$$\langle \delta \varepsilon_{11}^0 \delta \varepsilon_{22}^0 \rangle = \frac{1}{6} [(C_{11} - 3C_{12}) / (C_{11} - C_{12})(C_{11} + 2C_{12}) - 1/2C_{44}] kT/V_0 \quad (23)$$

$$\langle \delta \varepsilon_{12}^0 \delta \varepsilon_{12}^0 \rangle = \frac{1}{6} [1 / (C_{11} - C_{12}) + 3/4C_{44}] kT/V_0. \quad (24)$$

Here the quantities C_{ij} denote the elastic moduli of the cubic crystal in Voigt's notation, with $\frac{1}{3}(C_{11} + 2C_{12})$ denoting the bulk modulus $C^{(2)}$. With equations (21)–(24) we can calculate the stresses $\langle \sigma_{ij}(\mathbf{r}) \sigma_{kl}(\mathbf{r}) \rangle$ according to equation (15) and the strains $\langle \varepsilon_{ij}(\mathbf{r}) \varepsilon_{kl}(\mathbf{r}) \rangle$ via equation (16), yielding the invariants given by equations (1)–(4).

4. Results and discussion

In the following we consider the case of hypothetical pure amorphous iron, for which we can compare our results with those of computer simulations (see, e.g., Egami and Srolovitz 1982). For the calculations we need two sets of material parameters.

(1) The bulk and shear moduli K_0 and G_0 , entering equation (15), of the hypothetical homogeneous isotropic medium at that temperature for which we want to calculate the internal stresses in the amorphous material. As discussed in § 2 we may regard the volume average $\langle C_{ijkl}(\mathbf{r}) \rangle$ for the amorphous material as the elasticity tensor of this hypothetical medium, and we may yield this tensor in a simple model by averaging the elasticity tensor of the structural units over all orientations of the units. Assuming cubic symmetry of the units and inserting for the tensor components C_{11} , C_{12} and C_{44} in the local coordinate systems the values for iron at 300 K, we obtain $K_0 = 1.67 \times 10^{12}$ dyn cm⁻² and $G_0 = 8.92 \times 10^{11}$ dyn cm⁻².

(2) The bulk modulus $C^{(2)}$, or the tensor C_{ijkl} (C_{11} , C_{12} and C_{44} , respectively), entering equations (21)–(24), which describe the elastic properties of the isolated volume elements in the heat bath at the characteristic temperature T^c . When considering the isolated volume elements in the heat bath as liquid (case (i) of § 3), it is most reasonable to insert for T^c the melting temperature of iron, $T^c = 1807$ K. When assuming that the volume elements just before the freezing procedure are solid (case (ii) of § 3), it is more appropriate to identify T^c with the glass temperature of 760 K. To yield reasonable estimates for the elastic constants at these temperatures we have extrapolated the tabulated low-temperature values (Landolt-Börnstein 1979) in an appropriate manner (tables 1, 2).

The results for the invariants may be represented in the form $A(kT^c/V_0)$, where A is a respective prefactor (containing combinations of the two sets of material parameters), T^c is the characteristic temperature and V_0 is the volume of the isolated

Table 1. The calculated invariants at a temperature of 300 K for case (i), amorphous iron, for two different values of the characteristic temperature T^c .

T^c (K)	$C^{(2)}$ (dyn cm ⁻²)	$\sqrt{\langle p^2 \rangle}$ (eV Å ⁻³)	$\sqrt{\langle \tau^2 \rangle}$ (eV Å ⁻³)	$\sqrt{\langle l^2 \rangle}$	$\sqrt{\langle s^2 \rangle}$
760	1.59×10^{12}	0.0326	0.0282	0.0164	0.0306
1807	0.89×10^{12}	0.0672	0.0582	0.0339	0.0630

Table 2. The calculated invariants at a temperature of 300 K for case (ii), amorphous iron, for two different values of the characteristic temperature T^c .

T^c (K)	$C_{11}^{(2)}$ (dyn cm ⁻²)	$C_{12}^{(2)}$ (dyn cm ⁻²)	$C_{44}^{(2)}$ (dyn cm ⁻²)	$\sqrt{\langle p^2 \rangle}$ (eV Å ⁻³)	$\sqrt{\langle \tau^2 \rangle}$ (eV Å ⁻³)	$\sqrt{\langle I^2 \rangle}$	$\sqrt{\langle s^2 \rangle}$
760	2.00×10^{12}	1.38×10^{12}	1.05×10^{12}	0.0585	0.114	0.0226	0.190
1807	0.98×10^{12}	0.85×10^{12}	0.72×10^{12}	0.160	0.335	0.0574	0.558

units in the heat bath. In the following we insert for V_0 the atomic volume of crystalline iron, $V_0 = 11.7 \text{ \AA}^3$.

In tables 1 and 2 we report our results for the hydrostatic pressure p , the shear stress τ and the corresponding strains. For comparison, the above-quoted computer simulations for amorphous iron at zero temperature yield $\sqrt{\langle p^2 \rangle} = 0.064 \text{ eV \AA}^{-3}$ and $\sqrt{\langle \tau^2 \rangle} = 0.104 \text{ eV \AA}^{-3}$. These values are rather similar to our results when we insert as the characteristic temperature T^c the melting temperature in case (i) (liquid volume elements) or the glass temperature in case (ii) (solid units), as discussed above. The agreement must be considered as rather good in view of the fact that we have adopted some approximations, for instance the local continuum theory or the zeroth-order approximation for the perturbation theory. It should be noted that by our theory we can of course only calculate statistical averages for the stresses and strains, but not the stresses and site-symmetry coefficients (see, e.g., Egami *et al* 1980) at individual sites.

When inserting for K_0 and G_0 the values at the glass temperature instead of those at room temperature and adopting our case (ii), that is solid volume elements, we can also calculate the stress invariants at the glass transition and can compare the results with those obtained by molecular dynamics studies (Vitek *et al* 1984) and by a continuum model of the glass transition based on Eshelby's inclusion problem (Egami and Srolovitz 1982). As shown in table 3, the results of all three studies agree very well concerning the hydrostatic pressure $\sqrt{\langle p^2 \rangle}$. For the shear stresses $\sqrt{\langle \tau^2 \rangle}$, our result is similar to that of the molecular dynamics study, but differs by a factor of about two from the continuum result of Egami and Srolovitz (1982). Although, in view of the various approximations, the detailed numerical values of the continuum models should not be taken too literally, we want to elucidate the latter point further by comparing our approach with that of Egami and Srolovitz.

Both theories start from an ideal reference state without any internal stresses and introduce the internal stresses via incompatibilities. In our theory the incompatibilities are represented by the distribution of quasiplastic thermal strains ε_{ij}^Q that the isolated volume elements will exhibit in a heat bath at the glass transition temperature. For a given spatial distribution of quasiplastic strains we could in principle calculate the stress field $\sigma_{ij}(\mathbf{r})$ via equation (9), thereby taking into account all the elastic interactions between different sites. Of course we do not know the values of ε_{ij}^Q at the individual sites \mathbf{r} , but we have as statistical information just the correlation function $\langle \varepsilon_{mn}^Q(\mathbf{r}'') \varepsilon_{pq}^Q(\mathbf{r}''') \rangle$, which, according to equation (14), is given by the correlation function $g(\mathbf{r}'' - \mathbf{r}''')$ and by the statistical averages $\langle \varepsilon_{mn}^Q \rangle$ and $\langle \delta \varepsilon_{mn}^Q(\mathbf{r}) \delta \varepsilon_{pq}^Q(\mathbf{r}) \rangle$. From the correlation function for the quasiplastic strains we can calculate the statistical averages $\langle \sigma_{ij}(\mathbf{r}) \sigma_{kl}(\mathbf{r}') \rangle$ according to equation (13), which of course also contain elastic coupling effects between different sites. The averages $\langle \varepsilon_{mn}^Q \rangle$ and $\langle \delta \varepsilon_{mn}^Q(\mathbf{r}) \delta \varepsilon_{pq}^Q(\mathbf{r}) \rangle$ are calculated from Boltzmann statistics for the isolated volume elements. Statistical correlations between the fluctuations of the quasiplastic strains may be included in principle via the correlation function $g(\mathbf{r}'' - \mathbf{r}''')$,

Table 3. Comparison of the invariants at the glass temperature for amorphous iron, calculated in different theories. To obtain the final values, kT^c and V_0 must be inserted in units of eV and \AA^3 , respectively.

	$\sqrt{\langle p^2 \rangle} (\text{eV \AA}^{-3})$	$\sqrt{\langle \tau^2 \rangle} (\text{eV \AA}^{-3})$
Egami and Srolovitz (1982)	$0.653\sqrt{kT^c/V_0}$	$0.768\sqrt{kT^c/V_0}$
Vitek <i>et al</i> (1984)	$0.750\sqrt{kT^c/V_0}$	$1.298\sqrt{kT^c/V_0}$
Present paper	$0.806\sqrt{kT^c/V_0}$	$1.535\sqrt{kT^c/V_0}$

although in the zeroth-order approximation method for $\langle \sigma_{ij}(\mathbf{r})\sigma_{kl}(\mathbf{r}) \rangle$ the explicit form of this correlation function does not enter.

Obviously in our theory two types of correlations between different sites are included in principle, i.e. statistical correlations in the spatial distribution of quasiplastic strains via the function $g(\mathbf{r}'' - \mathbf{r}''')$ and elastic coupling effects between different sites via equation (9).

In their continuum theory of the glass transition, Egami and Srolovitz (1982) introduce the atomic-level stresses by a simple type of incompatibility, namely atoms which in an amorphous structure do not ideally fit into the environment as would be the case for a perfect crystal. The misfitting atom is modelled by an inclusion in a continuum. The total energy of the system is calculated with Eshelby's (1957) theory of inclusions as a sum of elastic energies associated with the local stresses σ_{ij} . It is assumed that the stress fluctuations are essentially independent of each other, that is any correlations between the various inclusions are neglected. The total energy expression contains only one set of material parameters, namely that of the amorphous system at the temperature considered. (It should be noted that in the paper by Egami and Srolovitz the zero-temperature elastic constants obtained from a computer model of amorphous iron are inserted instead of the values at the glass temperature, i.e. the temperature dependence of the elastic constants is neglected. In our theory two parameter sets are needed, that for the temperature considered and, for case (ii), that for the glass transition temperature. When considering the internal stresses at the glass transition itself, the two sets coincide.) Having determined in this way the total energy as a quadratic function of the independent local stresses, the thermal averages $\langle \sigma_{ij}\sigma_{kl} \rangle$ are calculated using Boltzmann's statistics, quite similar to our approach.

Obviously the main difference between the two theories concerns the inclusion of correlation effects between different sites in our theory. Perhaps this may explain the fact that our results are closer to the molecular dynamics results (Vitek *et al* 1984) than to those of Egami and Srolovitz (1982). However, one should also take into account, for a comparison of the continuum theories with the molecular dynamics study, that the latter results include dynamic fluctuations whereas the continuum theories assume a quasistatic state (Vitek *et al* 1984).

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