Molecular Dynamics Simulation on a Metallic Glass \( \text{Ni}_{0.2}\text{Zr}_{0.8} \)-System: Non-Ergodicity Parameter

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At the present paper we have computed non-ergodicity parameter from Molecular Dynamics (MD) Simulation data after the mode-coupling theory (MCT) for a glass transition. MCT of dense liquids marks the dynamic glass-transition through a critical temperature \( T_c \), that is reflected in the temperature-dependence of various physical quantities. Here, molecular dynamics simulations data of a model adapted to \( \text{Ni}_{0.2}\text{Zr}_{0.8} \) are analyzed to deduce \( T_c \) from the temperature-dependence of corresponding quantities and to check the consistency of the statements. Analyzed is the diffusion coefficients. The resulting values agree well with the critical temperature of the non-vanishing non-ergodicity parameter determined from the structure factors in the asymptotic solution of the mode-coupling theory with memory-kernels in “One-Loop” approximation.

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I. INTRODUCTION

The transition from a liquid to an amorphous solid that sometimes occurs upon cooling remains one of the largely unresolved problems of statistical physics \[1,2\]. At the experimental level, the so-called glass transition is generally associated with a sharp increase in the characteristic relaxation times of the system, and a concomitant departure of laboratory measurements from equilibrium. At the theoretical level, it has been proposed that the transition from a liquid to a glassy state is triggered by an underlying thermodynamic (equilibrium) transition \[3\]: in that view, an “ideal” glass transition is believed to occur at the so-called Kauzmann temperature, \( T_K \). At \( T_K \), it is proposed that only one minimum-energy basin of attraction is accessible to the system. One of the first arguments of this type is due to Gibbs and diMarzio \[3\], but more recent studies using replica methods have yielded evidence in support of such a transition in Lennard-Jones glass formers \[3,3\]. These observations have been called into question by experimental data and recent results of simulations of polydisperse hard-core disks, which have failed to detect any evidence of a thermodynamic transition up to extremely high packing fractions \[3\]. One of the questions that arises is therefore whether the discrepancies between the reported simulated behavior of hard-disk and soft-sphere systems is due to fundamental differences in the models, or whether they are a consequence of inappropriate sampling at low temperatures and high densities.

Different, alternative theoretical considerations have attempted to establish a connection between glass transition phenomena and the rapid increase in relaxation times that arises in the vicinity of a theoretical critical temperature (the so-called “mode-coupling” temperature, \( T_{MCT} \)), thereby giving rise to a “kinetic” or “dynamic” transition \[5\]. In recent years, both viewpoints have received some support from molecular simulations. Many of these simulations have been conducted in the context of models introduced by Stillinger and Weber and by Kob and Andersen \[6\]; such models have been employed in a number of studies that have helped shape our current views about the glass transition \[7\].

In the full MCT, the remainders of the transition and the value of \( T_c \) have to be evaluated, e.g., from the approach of the undercooled melt towards the idealized arrested state, either by analyzing the time and temperature dependence in the \( \beta \)-regime of the structural fluctuation dynamics \[15,16,17\] or by evaluating the temperature dependence of the so-called \( g_m \)-parameter \[18,19\]. There are further possibilities to estimates \( T_c \), e.g., from the temperature dependence of the diffusion coefficients or the relaxation time of the final \( \alpha \)-decay in the melt, as these quantities for \( T > T_c \) display a critical behaviour \( |T - T_c|^\beta \). However, only crude estimates of \( T_c \) can be obtained from these quantities, since near \( T_c \) the critical behaviour is masked by the effects of transversale currents and thermally activated matter transport, as mentioned above.

On the other hand, as emphasized and applied in \[20,21,22\], the value of \( T_c \) predicted by the idealized MCT can be calculated once the partial structure factors of the system and their temperature dependence are sufficiently well known. Besides temperature and particle concentration, the partial structure factors are the only significant quantities which enter the equations of the so-called non-ergodicity parameters of the system. The latter vanish identically for temperatures above \( T_c \) and their calculation thus allows a rather precise determination of the critical temperature predicted by the idealized theory.

At this stage it is tempting to consider how well the estimates of \( T_c \) from different approaches fit together and whether the \( T_c \) estimate from the non-ergodicity parameters of the idealized MCT compares to the values from the
full MCT. Regarding this, we here investigate a molecular dynamics (MD) simulation model adapted to the glass-forming Ni$_{0.2}$Zr$_{0.8}$ transition metal system. The Ni$_{x}$Zr$_{1-x}$ system is well studied by experiments and by MD-simulations as it is a rather interesting system whose components are important constituents of a number of multi-component ‘massive’ metallic glasses. In the present contribution we consider, in particular, the $x = 0.2$ compositions and concentrate on the determination of $T_c$ from evaluating and analyzing the non-ergodicity parameter, and the diffusion coefficients.

In the literature, similar comparison of $T_c$ estimates already exist for two systems. The studies come, however, to rather different conclusions. From MD-simulations for a soft spheres model, Barrat et al. find an agreement between the different $T_c$ estimates within about 15%. On the other hand, for a binary Lennard-Jones system, Nauroth and Kob get from their MD simulations a significant deviation between the $T_c$ estimates by about a factor of 2. Regarding this, the present investigation is aimed at clarifying the situation for at least one of the important metallic glass systems. Our paper is organized as follows: In Section II we present the model and give some details of the computations. Section III gives a brief discussion of some aspects of the mode coupling theory as used here. Results of our MD-simulations and their analysis are then presented and discussed in Section IV.

II. SIMULATIONS

The present simulations are carried out as state-of-the-art isothermal-isobaric $(N,T,p)$ calculations. The Newtonian equations of $N = 648$ atoms (130 Ni and 518 Zr) are numerically integrated by a fifth order predictor-corrector algorithm with time step $\Delta t = 2.5 \times 10^{-15}$s in a cubic volume with periodic boundary conditions and variable box length $L$. With regard to the electron theoretical description of the interatomic potentials in transition metal alloys by Hausleitner and Hafner, we model the interatomic couplings as in by a volume dependent electron-gas term $E_{\text{vd}}(V)$ and pair potentials $\phi(r)$ adapted to the equilibrium distance, depth, width, and zero of the Hausleitner-Hafner potentials for Ni$_{0.2}$Zr$_{0.8}$[31]. For this model simulations were started through heating a starting configuration up to 2000 K which leads to a homogeneous liquid state. The system then is cooled continuously to various annealing temperatures with cooling rate $-dT = 1.5 \times 10^{12}$ K/s. Afterwards the obtained configurations at various annealing temperatures (here 1500-800 K) are relaxed by carrying out additional isothermal annealing run at the selected temperature. Finally the time evolution of these relaxed configurations is modelled and analyzed. More details of the simulations are given in [31].

III. THEORY

In this section we provide some basic formulae that permit calculation of $T_c$ and the non-ergodicity parameters $f_i(q)$ for our system. A more detailed presentation may be found in Refs. [20, 21, 22, 32, 33]. The central object of the MCT are the partial intermediate scattering functions which are defined for a binary system by

$$F_{ij}(q,t) = \frac{1}{\sqrt{N_i N_j}} \langle \rho_i(q,t) \rho_j(q,0) \rangle$$

where

$$\rho_i(q) = \sum_{\alpha=1}^{N_i} e^{iq \cdot \vec{r}_i^{(a)}(t)}$$

is a Fourier component of the microscopic density of species $i$.

The diagonal terms $\alpha = \beta$ are denoted as the incoherent intermediate scattering function

$$F_i^s(q,t) = \frac{1}{N_i} \sum_{a=1}^{N_i} \langle \exp(iq \cdot \vec{r}_i^{(a)}(t) - \vec{r}_i^{(a)}(0)) \rangle$$

The normalized partial- and incoherent intermediate scattering functions are given by

$$\Phi_{ij}(q,t) = F_{ij}(q,t)/S_{ij}(q)$$

$$\Phi_i^s(q,t) = F_i^s(q,t)$$

where the $S_{ij}(q) = F_{ij}(q,t = 0)$ are the partial static structure factors.

The basic equations of the MCT are the set of nonlinear matrix integrodifferential equations given by

$$\ddot{\Phi}(q,t) + \Omega^2(q)\Phi(q,t) + \int_0^t d\tau M(q,t-\tau)\dot{\Phi}(q,\tau) = 0$$

where $\Phi$ is the $2 \times 2$ matrix consisting of the partial intermediate scattering functions $F_{ij}(q,t)$, and the frequency matrix $\Omega^2$ is given by

$$[\Omega^2(q)]_{ij} = q^2 k_B T \sum_k \delta_{ik} \left[S^{-1}(q)\right]_{kj}$$

$S(q)$ denotes the $2 \times 2$ matrix of the partial structure factors $S_{ij}(q)$, $x_i = N_i/N$ and $m_i$ means the atomic mass of the species $i$.

The MCT for the idealized glass transition predicts that the memory kernel $M$ can be expressed at long times
by
\[
M_{ij}(q,t) = \frac{k_B T}{2\rho m_i x_j} \int \frac{dk}{(2\pi)^3} \sum_{kl} \sum_{k'l'} V_{ikl}(q,k)V_{jl'k'}(q, q-k') \\
\times F_{kk'}(k,t)F_{ll'}(q-k, t),
\]
(8)
where \( \rho = N/V \) is the particle density and the vertex 
\( V_{\alpha\beta}(q,k) \) is given by
\[
V_{ikl}(q,k) = \frac{q \cdot k}{q} \delta_{ijl} c_{i\alpha}(k) + \frac{q \cdot (q-k)}{q} \delta_{ikl} c_{i\gamma}(q-k)
\]
(9)
and the matrix of the direct correlation function is defined by
\[
c_{ij}(q) = \frac{\delta_{ij}}{x_i} - [S^{-1}(q)]_{ij}.
\]
(10)
The equation of motion for \( F^s_i(q,t) \) has a similar form as eq. 6, but
the memory function for the incoherent intermediate scattering function is given by:
\[
M^s_i(q,t) = \int \frac{dk}{(2\pi)^3} \frac{1}{\rho} \left( \frac{q \cdot k}{q} \right) (cF)_i(k,t) \\
\times F^s_i(q-k, t),
\]
(11)
\[
(cF)_i(k,t) = (c_{ii}(q))^2 F_{ii}(q,t) + 2c_{ii}(q)c_{ij}(q) F_{ij}(q,t) \\
+ (c_{ij}(q))^2 F_{jj}(q,t) \quad j \neq i.
\]
(12)
In order to characterize the long time behaviour of the intermediate scattering function, the non-ergodicity parameters \( f(q) \) are introduced as
\[
f_{ij}(q) = \lim_{t \to \infty} \Phi_{ij}(q, t).
\]
(13)
These parameters are the solution of eqs. 11-12 at long times. The meaning of these parameters is the following: if \( f_{ij}(q) = 0 \), then the system is in a liquid state with density fluctuation correlations decaying at long times. If \( f_{ij}(q) > 0 \), the system is in an arrested, nonergodic state, where density fluctuation correlations are stable for all times. In order to compute \( f_{ij}(q) \), one can use the following iterative procedure [22]:
\[
f^{(l+1)}(q) = \frac{A(q) + B(q)}{C(q) + D(q)},
\]
(14)
where the matrix \( A(q), B(q), C(q), D(q), N(q) \) is given by
\[
A(q) = S(q) \cdot N[f^{(l)}, f^{(l)}](q) \cdot S(q),
\]
(15)
\[
B(q) = q^{-2} |S(q)||N[f^{(l)}, f^{(l)}](q)|S(q),
\]
(16)
\[
C(q) = q^2 + Tr(S(q) \cdot N[f^{(l)}, f^{(l)}](q)),
\]
(17)
\[
D(q) = q^{-2} |S(q)||N[f^{(l)}, f^{(l)}](q)|, \quad (18)
\]
\[
N_{ij}(q) = \frac{m_i}{x_i k_B T} M_{ij}(q).
\]
(19)
This iterative procedure, indeed, has two type of solutions, nontrivial ones with \( f(q) > 0 \) and trivial solutions \( f(q) = 0 \).

The incoherent non-ergodicity parameter \( f^s_i(q) \) can be evaluated by the following iterative procedure:
\[
q^2 \frac{f^{s,l+1}(q)}{1 - f^{s,l+1}(q)} = M^s_i[f, f^{s,l}](q).
\]
(20)
As indicated by eq. 15, computation of the incoherent non-ergodicity parameter \( f^s_i(q) \) demands that the coherent non-ergodicity parameters are determined in advance.

IV. RESULTS AND DISCUSSIONS

A. Partial structure factors and intermediate scattering functions

First we show the results of our simulations concerning the static properties of the system in terms of the partial structure factors \( S_{ij}(q) \) and partial correlation functions \( g_{ij}(r) \).

To compute the partial structure factors \( S_{ij}(q) \) for a binary system we use the following definition [23]
\[
S_{ij}(q) = \sum_{\alpha=1}^{N_i} \sum_{\beta=1}^{N_j} \frac{\delta(r - |r_\alpha(t) - r_\beta(t)|)}{N_i N_j}
\]
(21)
where
\[
g_{ij}(r) = \frac{V}{N_i N_j} \left( \sum_{\alpha=1}^{N_i} \sum_{\beta=1}^{N_j} \delta(r - |r_\alpha(t) - r_\beta(t)|) \right)
\]
(22)
are the partial pair correlation functions.

The MD simulations yield a periodic repetition of the atomic distributions with periodicity length \( L \). Truncation of the Fourier integral in Eq. 21 leads to an oscillatory behavior of the partial structure factors at small \( q \). In order to reduce the effects of this truncation, we compute from Eq. 22 the partial correlation functions for distance \( r \) up to \( R_c = 3/2L \). For numerical evaluation of eq. 21, a Gaussian type damping term is included
\[
S_{ij}(q) = \sum_{\alpha=1}^{N_i} \sum_{\beta=1}^{N_j} \frac{\delta(r - |r_\alpha(t) - r_\beta(t)|)}{N_i N_j}
\]
(23)
FIG. 1: Partial structure factors at $T = 1400$ K, 1300 K, 1200 K, 1100 K, 1000 K, 900 K and 800 K (from top to bottom): a) Ni-Ni-part, the curves are vertically shifted by 0.05 relative to each other; b) Ni-Zr-part, the curves are vertically shifted by 0.1 relative to each other; and c) Zr-Zr-part, the curves are vertically shifted by 0.5 relative to each other.

with $R = R_c/3$.

Fig. 1 shows the partial structure factors $S_{ij}(q)$ versus $q$ for all temperatures investigated. The figure indicates that the shape of $S_{ij}(q)$ depends weakly on temperature only and that, in particular, the positions of the first maximum and the first minimum in $S_{ij}(q)$ are more or less temperature independent.

In order to compare our calculated structure factors with experimental ones, we have determined the Faber-Ziman partial structure factors $a_{ij}(q)$ [37] and the Faber-Ziman total structure factor $S_{FZ \text{ tot}}(q)$ [36].

For a binary system with coherent scattering length $b_i$ of species $i$ the following relationship holds:

$$S_{FZ \text{ tot}}(q) = \frac{1}{b_i^2} \left[ b_1^2 a_{11}(q) + b_2^2 a_{22}(q) + 2 b_1 b_2 a_{12}(q) \right].$$

(25)

In the evaluation of $a_{ij}(q)$, we applied the same algorithm as for $S_{ij}(q)$. By using $a_{ij}(q)$ and with aids of the experimental data of the average scattering length $b$ one can compute the total structure factor. Here we take $b_i$ from the experimental data of Kuschke [23]. For natural Ni is $1.03 \times 10^{-12}$ cm and for Zr $0.716 \times 10^{-12}$ cm. Fig. 2 compares the results of our simulations with the experimental results by Kuschke [23] for the same alloy system at 1000 K. There is a good agreement between the experimental and the simulations results which demonstrates that our model is able to reproduce the steric relations of the considered system and the chemical order, as far is visible in the partial structure factors.

**B. Non-ergodicity parameters**

The non-ergodicity parameters are defined over Eq. 13 as a non-vanishing asymptotic solution of the MCT-eq. 6. Phenomenologically, they can be estimated by creating a master curve from the intermediate scattering functions with fixed scattering vector $q$ at different temperatures. The master curves are obtained by plotting the scattering functions $\Phi(q, t)$ as function of the normalized time $t/\tau_\alpha$.

Fig. 3 presents the estimated $q$-dependent non-ergodicity parameters from the coherent scattering functions of Ni and Zr, Fig. 4 those from the incoherent scattering functions. In Fig. 3 and 4 are also included the deduced Kohlrausch-Williams-Watts amplitudes $A(q)$ from...
the master curves and from the intermediate scattering functions at $T=1100$ K. (The further fit-parameters can be found in \[31\]).

In order to compute the non-ergodicity parameters $f_{ij}(q)$ analytically, we followed for our binary system the self-consistent method as formulated by Nauroth and Kob [22] and as sketched in Section III.A. Input data for our iterative determination of $f_{ij}(q) = F_{ij}(q, \infty)$ are the temperature dependent partial structure factors $S_{ij}(q)$ from the previous subsection. The iteration is started by arbitrarily setting $F_{Ni-Ni}(q, \infty)^{(0)} = 0.5S_{Ni-Ni}(q)$, $F_{Zr-Zr}(q, \infty)^{(0)} = 0.5S_{Zr-Zr}(q)$, $F_{Ni-Zr}(q, \infty)^{(0)} = 0$.

For $T > 1200$ K we always obtain the trivial solution $f_{ij}(q) = 0$ while at $T = 1100$ K and below we get stable non-vanishing $f_{ij}(q) > 0$. The stability of the non-vanishing solutions was tested for more than 3000 iteration steps. From this results we expect that $T_c$ for our system lies between 1100 and 1200 K. To estimate $T_c$ more precisely, we interpolated $S_{ij}(q)$ from our MD data for temperatures between 1100 and 1200 K by use of the algorithm of Press et.al. [33]. We observe that at $T = 1102$ K a non-trivial solution of $f_{ij}(q)$ can be found, but not at $T = 1105$ K and above. It means that the critical temperature $T_c$ for our system is around 1102 K. The non-trivial solutions $f_{ij}(q)$ for this temperature shall be denoted the critical non-ergodicity parameters $f_{cij}(q)$. They are included in Fig. 3. As can be seen from Fig. 3 the absolute values and the $q$-dependence of the calculated $f_{cij}(q)$ agree rather well with the estimates from the scattering functions master curve and, in particular, with the deduced Kohlrausch-Williams-Watts amplitudes $A(q)$ at 1100 K.

Fig. 4 shows the thus calculated diffusion coefficients of our Ni$_{0.2}$Zr$_{0.8}$ model for the temperature range between 800 and 2000 K. At temperatures above approximately 1250 K, the diffusion coefficients for both species run parallel with temperature in the Arrhenius plot, indicating

C. Diffusion-coefficient

From the simulated atomic motions in the computer experiments, the diffusion coefficients of the Ni and Zr species can be determined as the slope of the atomic mean square displacements in the asymptotic long-time limit

\[
D_i(T) = \lim_{t \to \infty} \frac{(1/N_i) \sum_{\alpha=1}^{N_i} |\mathbf{r}_{\alpha}(t) - \mathbf{r}_{\alpha}(0)|^2}{6t}.
\]  (26)
a fixed ratio $D_{Ni}/D_{Zr} \approx 2.5$ in this temperature regime. At lower temperatures, the Zr atoms have a lower mobility than the Ni atoms, yielding around 900 K a value of about 10 for $D_{Ni}/D_{Zr}$. That means, here the Ni atoms carry out a rather rapid motion within a relative immobile Zr matrix.

According to the MCT, above $T_c$ the diffusion coefficients follow a critical power law

$$D_i(T) \sim (T - T_c)^\gamma, \text{ for } T > T_c$$

with non-universal exponent $\gamma \approx 2.0$. In order to estimate $T_c$ from this relationship, we have adapted the critical power law by a least mean squares fit to the simulated diffusion data for 1050 K and above. The results of the fit are included in Fig. 3 by dashed lines. According to this fit, the system has a critical temperature of 950 K. The parameters $\gamma$ turn out as 1.8 for the Ni subsystem and 2.0 for the Zr system.

V. CONCLUSION

The results of our MD-simulations show that our system behave so as predicted by MCT in the sense that the diffusion coefficients follow the critical power law. After analyzing this coefficient we found that the system has critical temperature of 950 K.

Our analysis of the ergodic region ($T > T_c$) and of the non-ergodic region ($T < T_c$) lead to $T_c$ estimations which agree each other within 10 %. These $T_c$ estimations are also in acceptable compliance with the $T_c$ estimation from the dynamic phenomenons. Within the scope of the precision of our analysis, the critical temperature $T_c$ of our system is about 1000 K.

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