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# From metallic glasses to nanocrystals: Molecular dynamics simulations on the crossover from glass-like to grain-boundary-mediated deformation behaviour

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## ABSTRACT

Nanocrystalline metals contain a large fraction of high-energy grain boundaries, which may be considered as glassy phases. Consequently, with decreasing grain size, a crossover in the deformation behaviour of nanocrystals to that of metallic glasses has been proposed. Here, we study this crossover using molecular dynamics simulations on bulk glasses, glass–crystal nanocomposites, and nanocrystals of  $\text{Cu}_{64}\text{Zr}_{36}$  with varying crystalline volume fractions induced by long-time thermal annealing. We find that the grain boundary phase behaves like a metallic glass under constraint from the abutting crystallites. The transition from glass-like to grain-boundary-mediated plasticity can be classified into three regimes: (1) For low crystalline volume fractions, the system resembles a glass–crystal composite and plastic flow is localised in the amorphous phase; (2) with increasing crystalline volume fraction, clusters of crystallites become jammed and the mechanical response depends critically on the relaxation state of the glassy grain boundaries; (3) at grain sizes  $\geq 10$  nm, the system is jammed completely, prohibiting pure grain-boundary plasticity and instead leading to co-deformation. We observe an inverse Hall–Petch effect only in the second regime when the grain boundary is not deeply relaxed. Experimental results with different grain boundary states are therefore not directly comparable in this regime.

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## 1. Introduction

Deformation mechanisms operating in nanocrystalline metals sensitively depend on the average grain size and grain size distribution [1]. In contrast to coarse-grained polycrystalline metals, where plastic strain is predominantly carried by dislocations, grain-boundary-mediated deformation processes (including sliding and shuffling mechanisms) become increasingly relevant with decreasing grain size. Since the first controlled synthesis of nanocrystalline metals in the late 1980s [2], a large body of literature on the nature of deformation mechanisms in this material class has appeared, which eventually led to the development of deformation maps showing active mechanisms as a function of grain size, temperature, or strain rate (see Ref. [3] for an overview). Since low-

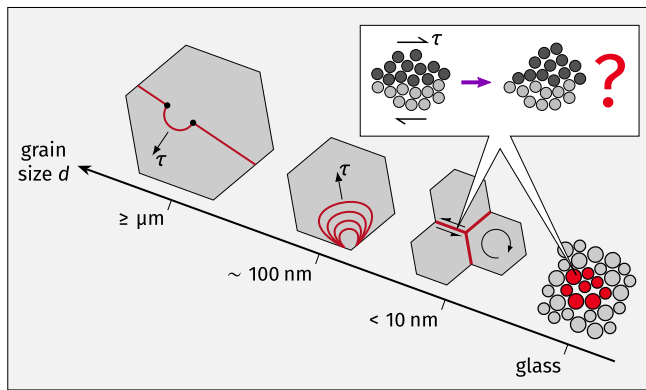
energy grain boundaries are typically absent in nanocrystalline microstructures [3], several studies have fostered the view that a nanocrystalline metal could also be considered as a composite of a glassy, percolating grain boundary phase confined between nanocrystallites [4,5]. Thus, a smooth transition to glass-like deformation behaviour could be expected with decreasing grain size (see Fig. 1).

The parallels between grain boundary deformation and the deformation mechanisms in metallic glasses (MGs) are indeed striking: MGs deform via shear-transformation zones (STZs), small regions in which a shear deformation is activated under external stress [6,7]. Similar concepts have been applied to grain boundaries [8,9] and yielding in nanocrystals has been shown to exhibit a  $T^{2/3}$  temperature dependence [10], just as described for MGs by Johnson and Samwer [11]. Trelewicz and Schuh performed nanoindentation experiments on very small-grained Ni–W alloys and found that they show pop-in events similar to those observed in indentation on metallic glasses [5]. Moreover, the indents featured shear offsets in the surrounding pile-up, indicative of shear banding. An extrapolation of these indentation testing data with varying grain sizes arrives at the amorphous limit [5,12,13], estimated at around

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**Fig. 1.** Transition from nanocrystals to metallic glasses. While coarse-grained polycrystals exhibit classical, bulk-like dislocation activity, deformation mechanisms in nanocrystals depend on the average grain size. Grain boundaries act as sinks and sources for dislocation activity, and the plasticity of the grain boundaries themselves becomes important in the sub-10-nm regime. With further decrease of the grain size  $d$ , a transition to deformation behaviour known from glasses was postulated: Experimental data indicate similarities between shear transformations in glasses and grain boundary plasticity, suggesting a smooth transition to the glassy state at small  $d$ .

1 nm and supported by simulations that report a collapse of the crystalline lattice at such small grain sizes [14–16]. It was also conclusively shown by experiment and computer simulations that the grain boundary phase is characterised by a lower shear modulus, which starts affecting the effective macroscopic shear modulus [17,18], making the structure reminiscent of the liquid-like/solid-like division in metallic glasses [19–22].

A problem with the experimental data, which was mostly obtained for Ni–W systems, is that the grain size can only be controlled by varying the tungsten content [5,12,13]. Pure systems exhibit rapid grain growth even at room temperature [23,24]. By segregation of solutes to the grain boundaries, small grain sizes can be stabilised [13,25–30], even in miscible systems [31,32]. As a result, though, not only the grain size but also the nature of the grain boundary itself may be modified [30,33–37]. Therefore, any quantitative trend extracted experimentally from varying grain sizes below 10 nm has to be interpreted with care, since the grain boundary state and composition also changes with grain size.

If we accept at this point the proposition of glass-like grain boundaries, we could also consider a nanocrystal as one limit of a glass–crystal nanocomposite. Such composites have received a lot of attention for their potential to retain the high yield strength and large elastic limit of MGs, while improving their ductility. It is generally found that secondary phases enhance the tendency for shear band nucleation and lead to a more homogeneous strain distribution [38–41]. Regarding the interaction of propagating shear bands with precipitates, small precipitates can be avoided (“wrapped”) by shear bands [42], leaving the crystalline phase undeformed [43]. Bigger precipitates block the shear band propagation or co-deform with the glass matrix [42,43]. These investigations are mostly concerned with smaller volume fractions of crystalline phase, though, and it is unclear if they also apply to nanocrystalline metals.

The purpose of the present work is to study the crossover from glass–crystal nanocomposites to nanocrystals using molecular dynamics (MD) computer simulations. We use the well-established MG  $\text{Cu}_{64}\text{Zr}_{36}$  with embedded brittle Laves phase nanocrystallites as a model system. The advantage over studying ductile nanocrystallites is that the plastic response of the system is exclusively carried by the glassy phase/grain boundaries and thus we can disentangle the grain boundary activity from dislocation activity. As was recently shown [44–46], Laves crystallites can be grown in MD simulations using the Finnis–Sinclair-type potential by Mendelev

[47]. This opens the possibility of growing crystallites in a system of constant composition, thereby obtaining samples ranging from a homogeneous MG, over glass–crystal composites, to nanocrystals.

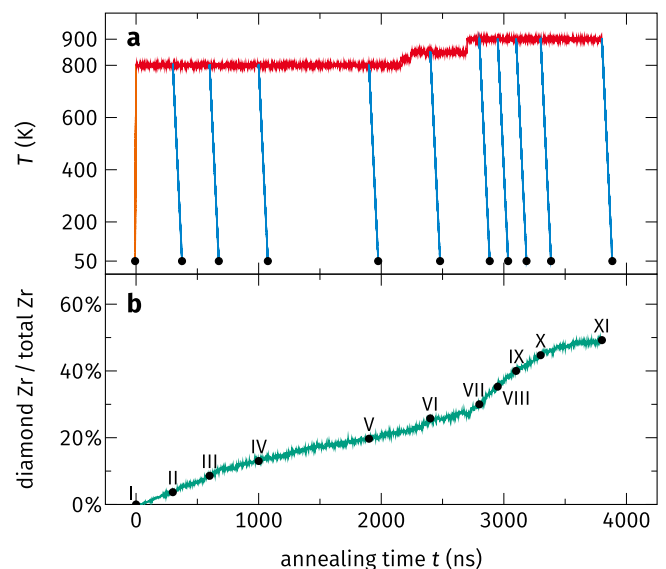
## 2. Computational methods and analysis

All MD simulations were performed with Cu–Zr systems using LAMMPS [48] and the Finnis–Sinclair-type potential by Mendelev et al. [47]. The integration time step was 2 fs in all cases.

### 2.1. Synthesis and annealing procedure

A  $\text{Cu}_{64}\text{Zr}_{36}$  metallic glass consisting of  $N = 63,108$  atoms was quenched from the melt down to 50 K with a cooling rate of 0.01 K/ps and equilibrated there for 2 ns. This “as-quenched” sample is designated sample I and has dimensions of around  $10 \times 10 \times 10 \text{ nm}^3$ . In order to facilitate the crystallisation of  $\text{Cu}_2\text{Zr}$  Laves phases [46], we heated the glass to 800 K (which is close to the glass transition  $T_g$  [47]) with  $\dot{T} = 0.1 \text{ K/ps}$ . We held the glass at this temperature for roughly 2  $\mu\text{s}$  and then increased the temperature step-wise to 850 K and then to 900 K to speed up the crystallisation kinetics. Fig. 2 shows the complete annealing procedure. Neither a glass transition nor melting were observed; indeed the glass transition temperature rises with annealing time (see Appendix A). At intermediate steps, snapshots of the simulation were taken and cooled with  $\dot{T} = 0.01 \text{ K/ps}$  back to 50 K. These snapshots with different crystalline volume fractions are labelled as sample II–XI. We detected the presence of crystallites and computed the grain sizes as described in Appendix B and found a mix of C14 and C15 Laves phases [49] with an amorphous grain boundary. Details about the nucleation of crystallites are provided in Appendix C.

For later mechanical testing, these samples were replicated  $3 \times 1 \times 7$  times to obtain specimen of  $30 \times 10 \times 70 \text{ nm}^3$  size. Open boundaries were introduced in  $x$  direction to increase the tendency for shear localisation as discussed in Ref. 40. The samples were then equilibrated at target temperatures of 50 K and 250 K for 1 ns. The structural, thermodynamic, and elastic properties were determined



**Fig. 2.** The annealing procedure. (a) Temperature profile. The sample is heated with 0.1 K/ps to 800 K. After around 2  $\mu\text{s}$  the temperature is increased step-wise to increase the crystallisation rate. Snapshots are taken at intervals and cooled down with 0.01 K/ps. (b) The fraction of zirconium atoms in diamond superlattice configurations as a function of annealing time as a rough indicator of crystalline volume fraction. The snapshots are labelled I–XI.

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