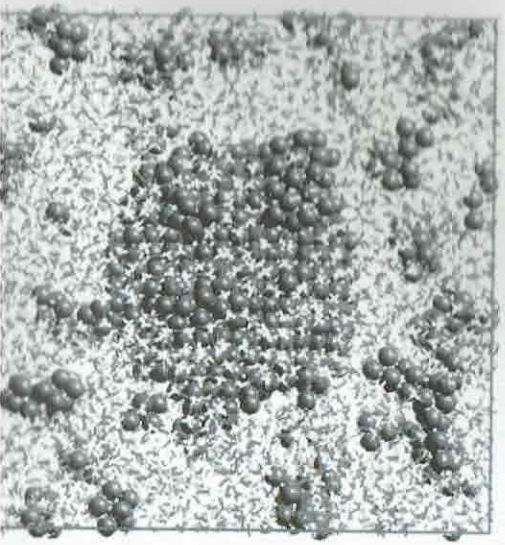
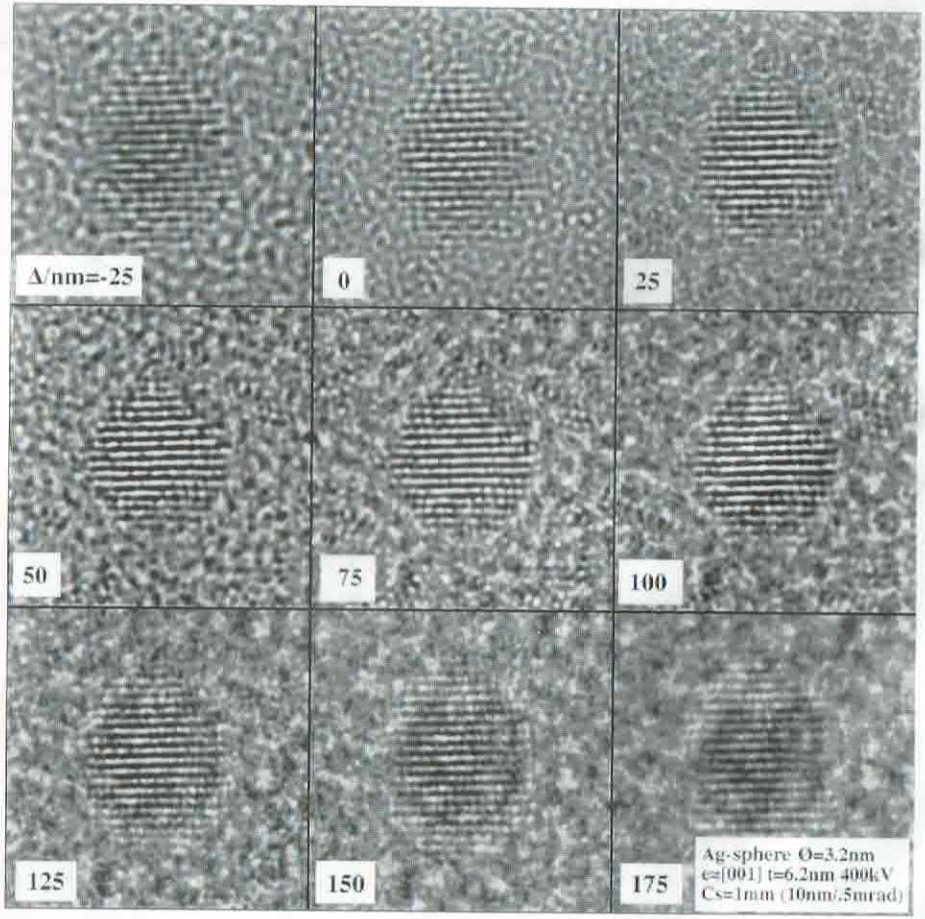


Fig. 3: Spherical Ag-particle (1048 atoms, ø=3.2nm) in 30% Na-Ag ion-exchanged sodium silicate glass after MD annealing cycle: 300K-1000K-300K in 50ps

Fig. 4: Simulated HREM defocus series of the annealed Ag-particle in glass:
Imaging conditions:
U=400kV, Cs=1mm, ∆=10 nm, α=0.5mrad



Molecular Dynamics Structure Simulations of Ag Particles in Glass for HREM

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g particles in sodium silicate glass are described and analyzed by classical molecular dynamics simulations. The resulting structures are the basis for the interpretation of high resolution electron microscope (HREM) investigations.

1. Introduction

Metallic particles embedded in glass strongly influence the optical, mechanical, and electrical properties of the latter, emphasizing the importance of HREM investigations, which provide structural information at the atomic level [1,2]. The particles are mostly generated by sodium-silver ion exchange and subsequent annealing to control migration and clustering. Molecular dynamics simulations are applied to generate suitable models to simulate HREM micrographs and to analyze measured lattice parameter variations [3-5].

2. Molecular Dynamics Structure Simulations of Sodium Silicate Glasses

To establish a realistic glass model requires an amorphous structure with a crystalline local atomic environment, but a correlation of the atomic positions vanishing over far distances, and special topological rules. Different strategies of the glass generation starting with a α-$Na_2Si_2O_5$ crystal are considered using the Cerius program package [6] and a modified program of the Rutgers State University [7]. For the MD calculations the modified Born-Mayer-Huggins (BMH) pair potential is used including Stillinger-Weber angular terms for covalent glass bondings and an embedded atomic potential (EAM) [8] describing the metallic interactions.

Fig. 1a shows a MD generated glass, with two annealing cycles being applied: First, the crystalline density is reduced to ρ=1.0g/cm^3, MD cycle 300K - 8000K - 100K in 100ps; second, the density is set according to the glass density ρ=2.5g/cm^3, MD cycle 300K - 4000K - 100K in 100ps. The corresponding pair distribution functions (PDF) and angular distributions in Fig. 1b,c demonstrate that the local atomic environment is sufficiently described. Relative to the peaks of the crystal those of the glass structure are lowered and broadened, revealing a correlation of the atomic positions solely for small distances.

articles in Glass

ms are built into the sodium silicate glass in different ways. First, crystalline Ag s of different shape and size were included into the enlarged sodium silicate glass the relaxation behaviour of the precipitates was investigated [5]. Second, some of the atoms were randomly replaced by silver. A subsequent annealing process caused a n of the Ag atoms, resulting in a clustering process of these atoms strongly depending nnealing temperature (Fig. 2), the ion exchange rate, and on the Ag - Ag as well as the ss pair potential chosen. Detailed results will be published elsewhere.
hows a spherical Ag particle embedded in an ion-exchanged glass matrix after 100ps ulation (300K - 1000K - 300K). Besides the enlargement of the particle introduced e many small clusters of up to 50 atoms grown during annealing.

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micrographs are simulated for Ag particles of different orientation and relaxation state ed into sodium silicate glass. While particle rotation solely causes minor changes of ce fringe distances, the relaxation behaviour is clearly revealed by HREM [5]. Based tructural model given in Fig. 3 a computer simulated HREM defocus series (Fig. 4) is ed. The changes of the particle surface indicating the particle growth will be imaged Besides, near the Scherzer focus there are contrast correlations that are caused by a nall Ag clusters.

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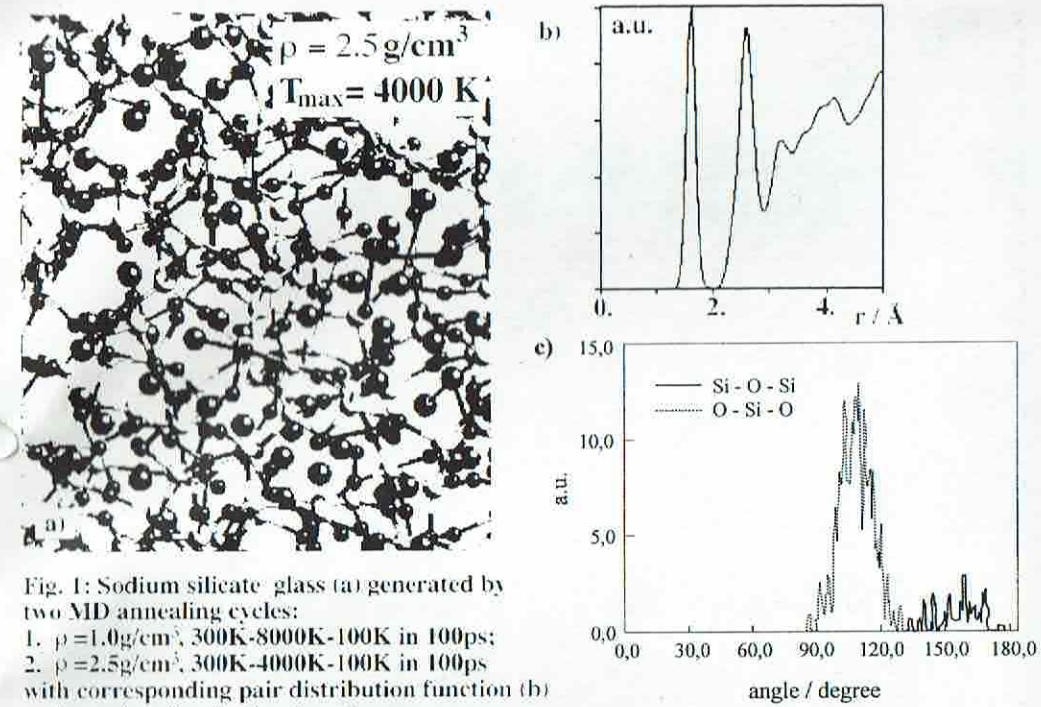

Fig. 1: Sodium silicate glass (a) generated by two MD annealing cycles:
1. ρ =1.0g/cm³, 300K-8000K-100K in 100ps;
2. ρ =2.5g/cm³, 300K-4000K-100K in 100ps
with corresponding pair distribution function (b) and angular distribution function (c)

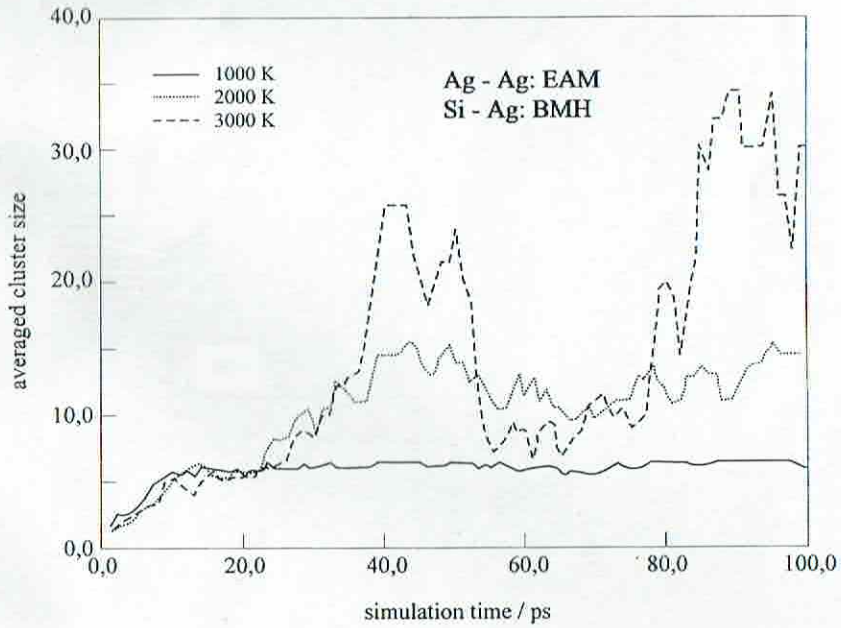

Fig. 2: Averaged cluster size vs. simulation time for different annealing temperatures for 30 % Na-Ag ion-exchanged sodium silicate glass