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Defect Dynamics in the Network Glass SiO_2[1] KATHARINA VOLLMAYR-LEE, Bucknell University, USA, ANNETTE ZIPPELIUS, Georg-August-University Goettingen, Germany — We study the dynamics of the strong glass former SiO_2 via molecular dynamics simulations below the glass transition temperature. To focus on microscopic processes, we average single particle trajectories over time windows of about 100 particle oscillations. The structure on this coarse-grained time scale is very well defined in terms of coordination numbers, allowing us to identify ill-coordinated atoms, called defects in the following. The most numerous defects are O-O neighbors, whose lifetimes are comparable to the equilibration time at low temperature. On the other hand SiO and OSi defects are very rare and short lived. The lifetime of defects is found to be strongly temperature dependent, consistent with activated processes. Single-particle jumps give rise to local structural rearrangements. We show that in SiO_2 these structural rearrangements are coupled to the creation or annihilation of defects, giving rise to very strong correlations of jumping atoms and defects.

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