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Defect diffusion in CaF_2 for optical applications RIX STEPHAN, SCHOTT AG, Mainz, Germany and Johannes Gutenberg-Universität Mainz, Germany, UTE NATURA, SCHOTT AG, Division Schott Lithotec, Jena, Germany, MARTIN LETZ, SCHOTT AG, Mainz, Germany, LUTZ PARTHIER, SCHOTT AG, Division Schott Lithotec, Jena, Germany, CLAUDIA FELSER, Institute for Anorganic and Analytical Chemistry, Johannes Gutenberg-Universität Mainz, Germany — Single crystal calcium fluoride (CaF_2) is an important lens material for deep-ultraviolet optics and a key material for 193 nm lithography. The exposure to high radiation densities requires extreme laser-stability of the material, which is to a large part ensured by a high purity level. However, for long exposure times the optical quality of CaF_2 is affected by radiation-induced point defects, namely F- and H-centers. The migration and agglomeration of these point defects play an important role in understanding laser-damage processes on a microscopic level. We use ab-initio methods to investigate the stabilization of laser-induced point defects. As stabilization processes involve defect migration, we also focus on diffusion properties of defects. We present results for the diffusion barrier and details of the transition state of the migrating F-center, which shows good agreement with experimental results.

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