Atomistic modelling of Si and C migration at (0001) sufrace of SiC crystal.

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Resume : Diffusion and desorption of C and Si atoms on (0001) surfaces of 4H Silicon Carbide have been studied by means of atomistic modeling. Atomic interactions were described by many-body Analytic Bond-Order Potentials . Migration activation barriers have been determined using Nudged Elastic Band - Climbing Image algorithm applied with Quenched Molecular Dynamics based on Velocity Verlet algorithm. The shape (with characteristic twin peaks) and values of migration barriers show good agreement with published experimental data and ab-initio calculations. Obtained results, crucial for crystal growth and refinement processes, point out on several important issues: (i) diffusion and desorption of C atoms present similar barrier values indicating lack of C migration on C surface, (ii) relatively low Si diffusion barriers show preferences for Si atoms to migrate on both C and Si free surfaces. These are preliminary results, further research including application of the barriers into KMC simulations is in progress.

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