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In material manufacturing it is usually impossible to discriminate between the role and weight of each factor that may affect the structure composition at nanoscopic scale. This gap can be filled by computational modeling techniques and methods. One of the most powerful is the molecular dynamics (MD), which provides detailed information on the effect of substitutional disorder, defects, vacancies, pressure or temperature onto the manufacturing process, and allows to isolate and control the parameters and conditions for manufacturing.

We will present here our data on Al2O3 and grAl structures that resulted from the QuCos project activities.