Computational analysis of precipitates, parasitic deposits and gas-to-particle conversion during Cz and DS Si-crystal growth.

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The present paper focuses on modeling Cz and DS Si-crystal growth. There are a few related problems in the performance of these technologies. We will emphasize three of them. First, impurities contained in silicon feedstock and generated due to the melt-to-crucible contact strongly affect the efficiency of mono and multicrystalline silicon solar cells. Oxygen and nitrogen are mainly coming from quartz crucible wall and crucible coating, while the main sources for carbon are feedstock and graphite furnace elements. Carbon, nitrogen and oxygen dissolved in the melt interact with silicon and each other, generating such precipitates as SiC, Si₃N₄ and Si₂N₂O [1], [2]. Second, oxygen is mostly evacuated through the free melt surface and transported as silicon monoxide by argon flow downstream to the reactor outlet. Therewith, SiO-vapor chemically reacts with graphite elements, supplying such by-products as CO and Si in the gaseous phase. In turn, SiO, CO and Si become sources of SiC- and Si-parasitic deposits on hot elements of reactor, shortening significantly, in particular, the heater lifetime. Moreover, SiO₂ or SiO can be deposited on the cold surfaces [3]. Third, SiO-vapor in some cooled regions, e.g., in outlet tubes and near upper part of the heat shield around the crystal turns out to be supersaturated and converted into SiO-particles in the gas-phase. Their entry into the silicon melt may cause single crystal structure loss [3]. In this connection, the conventional heat and mass transport model [4] is extended to describe those phenomena. The model is verified by comparing our computations with available experimental data. It is found for the DS method that maximum amount of Si₃N₄-precipitates is predicted near the crystal top where the nitrogen percentage is higher due to absence of its loss at melt free surface. As contrasted to Si₃N₄-precipitates, Si₂N₂O-concentration reaches its maximum near the crystal bottom. Obviously, its formation then is controlled primarily by the oxygen decreasing with the height. Therewith, in both cases the precipitates are accumulated along the crystal center. SiC-concentration exhibits a behavior similar to that of Si₃N₄ for the same reasons but is remarkably less localized near the crystal center. Accounting for the lack of detailed information on the process parameters and the reactor design, our computations qualitatively agree well with experimental data presented in [5]. The developed chemistry is applied to modeling the Cz silicon growth for a 155-mm-diameter ingot in a Kayex CG6000 puller [3]. As it follows from our computations, a zone near the shield top is inconsiderably heated, and our model predicts SiO₂-deposit on upper part of the shield where it is just observed in experiment. In addition, SiO-vapor is supersaturated here and, hence, converted into the particles. Further, SiO is transported downstream where it interacts with the hot graphite heater. As it follows from our simulation, Si-deposit of a short length is formed in region of relatively low temperature at the top and bottom of heater, while a central part is coated by silicon carbide. Their formation is accompanied by graphite etching. The same computation is performed for an optimized design of the furnace where the outlet is located opposite to the upper part of crucible, and insulation is added at the top of molybdenum shield. Our computations show that modification of the hot zone near the shield could help to suppress SiO-supersaturation. Also Si- and SiC-deposition rate on the
shield and on the heater is predicted to be negligibly low due to the alternative location of reactor outlet. The results obtained are well consistent with experimental data [3].

To conclude, the advanced chemistry model for DS and Cz Si-crystal growth is developed to account for precipitation in the melt and parasitic deposits from the gas phase as well as gas-to-particle conversion. The software tool, CGSim crystal growth simulator, based on the model allows optimization of reactor design and process conditions to avoid the gas-phase condensation and to minimize the parasitic deposits.

References