MODEL CALCULATIONS OF EVAPORATION OF CAI-LIKE MELTS ENRICHED IN TiO₂. M. A. Ivanova^{1,2}, S. I. Shornikov¹, K. M. Ryazantsev¹, R. A. Mendybaev³, and G. J. MacPherson². ¹Vernadsky Institute, Kosygin St. 19, Moscow 119991, e-mail: ivanovama@si.edu; ²Department of Mineral Sciences, National Museum of Natural History, Smithsonian Institution, Washington, DC. 20560, e-mail: MacPhers@si.edu; ³Department of the Geophysical Sciences, University of Chicago, Chicago, IL 60637, e-mail: ramendyb@uchicago.edu

Introduction: Ca-, Al-rich Inclusions (CAIs) record the cumulative effects of high-temperature volatility-controlled processes during the first several million years of solar system history [1]. The most important processes in CAIs formation are condensation, melting and evaporation. We recently presented results on thermodynamic modeling of evaporation of CAI-like melts with different compositions from CV3 chondrites [2]. The modeling, confirmed by experiments [3], showed that evaporation of a spinel-rich and CaO-poor CAI composition melt (5aN) with CaO/Al₂O₃ ratio ~ 0.3 results in a compositional trend that well fits the compositions of refractory hibonite-rich CAIs from CH-CB chondrites [2, 3]. Similar results were obtained during thermodynamic modeling of evaporation of two spinel-melilite-hibonite-rich CAIs 54E (fine-grained; CaO/Al₂O₃ ~0.3) and 48E (texturally similar to Compact Type As; CaO/Al₂O₃ ~solar) with bulk chemical compositions of typical hibonite-rich CAIs [4]. The compositions studied previously did not include Ti, which is one of the major element in CAIs, and thus could potentially affect evaporation trajectories. Here we report results of theoretical modeling of evaporation of TiO2-rich CAIs melts with initially different TiO₂ contents, to investigate titanium behavior during evaporation, and how titanium affects the compositional trends of evaporative residues after crystallization.

Results: The calculations of the evaporation trends have been conducted at 2173K using the semi-empirical model of thermodynamic codes developed by [5]. The model is based on the theory of associated solutions and on experimentally determined activities of melt components in CaO-MgO-FeO-Al₂O₃-TiO₂-SiO₂ system determined by the Knudsen mass spectrometric effusion method in the temperature range of 1600-2500 K.

As the starting material in the modeling chemical compositions of several CAIs with different TiO₂ content have been used (Table 1). We chose CAIs of two populations — enriched in Al₂O₃ with non-solar CaO/Al₂O₃ ratio (~0.3) and CAIs with solar CaO/Al₂O₃ ratio (~1). CAIs *E005*, *E007*, *E354* and *E377* are from CH chondrite NWA 470, but CAIs enclosed on amoeboid olivine aggregates (AOAs) *35E* and *52E* as well as CAIs *6aN* and *40E-1* are from CV3 chondrites NWA 3118 and Efremovka. Compositional trends of evaporative residues after crystallization are shown on plots (Fig. 1).

Discussions: As it was shown earlier [6] evaporation of CAI-like melts starts with fast loss of FeO, followed by MgO and SiO₂ resulting in enrichments of refractory Al₂O₃ and CaO in the residual melt. Later CaO could also evaporate, unless TiO₂ is present in the melt causing CaO to be retained due to its affinity with TiO₂ (perovskite compositional affinity) [6]. Despite variations in the CAIs' initial melt compositions (Table. 1), there is a certain general similarity in the change of the ratio of the most refractory components (CaO and Al₂O₃) in the residual melts during evaporation.

However, the calculation showed that TiO2 content in CAI melts has very little, if any, affect on general compositional trends of evaporation residues. We observed similar tendency in changing of chemical compositions which we have been reported recently [2-4]. Evaporation of CV3 CAI in AOA 35E melt (initial composition within the anorthite stability field) results in compositions typical for CH-CB hibonite- and grossite-bearing CAIs is due to its initial high Al₂O₃ content and low CaO/Al₂O₃ ratio of ~0.3. As the CaO/Al₂O₃ ratio in starting materials increases (to 0.6 in CAI in AOA 52E, to 0.7 in 6aN, and to 1.2 in 40E-1) the evaporation trajectories trend away from the field of refractory CAIs of CH-CBs (Fig. 1). Evaporation of CH CAIs melts (E007, E377) with CaO/Al₂O₃ ratio ~ 0.3 and > 0.3 also results in very refractory inclusions in the range of CH CAIs compositions. Initial compositions of these CAIs are already within the hibonite stability field (E007) and out of the diagram, in CH CAIs compositions (E377, E005, E354). Trend of 40E-1 is unique, because this CAI is enriched in CaO with a high ratio Ca/Ti in initial composition.

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References: [1] MacPherson G. J. (2014) In: Meteorites and Cosmochemical Processes (Ed. A. M. Davis), Vol. 1. Treatise on Geochemistry, 2nd ed., 139–179. [2] Ivanova M. A. et al. (2017) LPS XLVIII, Abs. #1363. [3] Ivanova M. A. et al. (2018) LPS XLIX, Abs. #1965. [4] Ivanova M. A. et al. (2018) Meteorities & Planet. Sci 53, abstract #6070; [5] Shornikov S. I. et al. (2017) LPS XLVIII. Abs. #1134. [6] Shornikov S. I. et al. (2015) International Conf. XVI, Physico-chemistry and Petrology in the Earth Sciences, 281–284.

Table 1 Initial	bulk chemica	1 compositions	of investigated	CAIs before ev	aporation (wt.%).
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CH chondrite	CaO	MgO	Al ₂ O ₃	FeO	TiO ₂	SiO_2	CaO/Al ₂ O ₃	MgO/SiO ₂
CAI <i>E007</i>	17.81	8.30	51.32	0.56	3.60	18.41	0.35	0.45
CAI <i>E005</i>	30.41	0.10	57.02	0.00	6.37	6.10	0.53	0.02
CAI <i>E354</i>	26.91	2.00	58.33	0.68	7.37	4.71	0.46	0.42
CAI <i>E377</i>	10.88	17.20	60.63	0.56	9.53	1.21	0.18	14.21
CV3 chondrites	CaO	MgO	Al ₂ O ₃	FeO	TiO ₂	SiO ₂	CaO/Al ₂ O ₃	MgO/SiO ₂
CAI 6aN	29.04	8.42	39.40	1.50	2.25	19.39	0.74	0.43
CAI in AOA 52E	14.17	23.35	23.54	0.86	5.99	32.08	0.60	0.73
CAI in AOA 35E	10.69	18.86	43.86	2.00	7.01	17.57	0.24	1.07
CAI 40E-1	36.38	4.26	29.87	0.40	8.63	20.47	1.22	0.21

