CLUSTER ANALYSIS AND CLASSIFICATION OF PRESOLAR SILICON CARBIDE GRAINS.

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Introduction: The discovery of stardust in the mid-1980s has led to a major breakthrough in our understanding of physical and chemical processes occurring in stars. These presolar grains are recognizable by their significant deviations in isotopic compositions from material formed in the Solar System, which are also proof of their stellar origin. Among the different types of stellar minerals, SiC grains were extensively studied, because of their easy extraction during acid dissolution and their relatively large sizes, especially in the Murchison meteorite.

The isotopic compositions of presolar grains are usually compared with astrophysical models and observations to assess their provenance and define different groups of grains. For instance, most SiC condensed in AGB stars (~95%) and supernovae (<5%) [e.g., 1]. The classification of presolar SiC grains is however continuously evolving due to advances in measurements of isotopic compositions of a variety of elements and in modeling stellar evolution and nucleosynthesis. The presence of a presolar grain database (PGD) [2] and its current update [3] provides an opportunity to evaluate the classification of SiC presolar grains using state-of-the-art statistical approaches. Indeed, advances in machine learning algorithms and their application to mineralogy are currently improving mineral classification systems and the identification of formation environments [4]. Here, we use a data-driven approach to evaluate the classification of presolar SiC grains, using cluster analysis.

Methods: We used the updated PGD presented at this meeting [3] on SiC presolar grains (version PGD_SiC_2020-01-03). Since studies on SiC provide isotopic compositions of a selection of elements, we used different subsets of the database, having different numbers of observations and attributes, including C, N, Si, Ti, and Al isotopic compositions. Here, we present clustering results for a dataset of ~1700 observations of the four attributes $^{12}C/^{13}C$, $^{14}N/^{15}N$, $\delta^{29}Si$, and $\delta^{30}Si$. In order to homogenize units, isotopic compositions expressed in delta form were converted into isotopic ratios and all isotopic ratios were converted into log units and then normalized to a same average and standard deviation. Cluster analysis was conducted with a model-based clustering algorithm, with the R package *mclust*, which is based on the assumption that the dataset is a Gaussian finite mixture.

Results: We conducted a principal component analysis collapsing the dimensions into more significant ones (Fig. 1). It shows that 68 and 18 % of the variance of the dataset is explained by the first and second components, respectively.

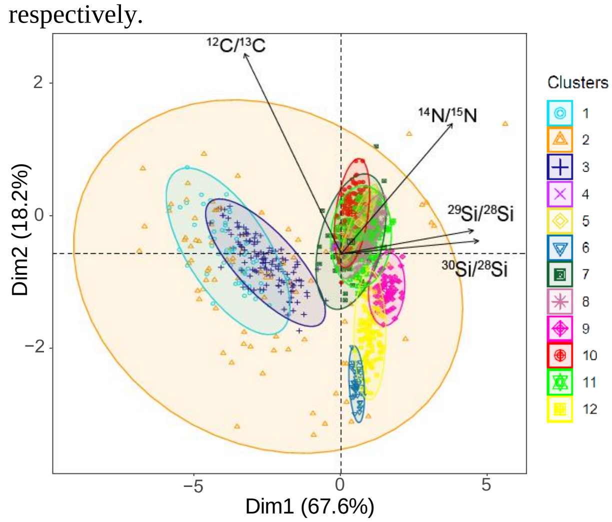

Fig. 1: Principal component analysis biplot for presolar SiC grains using data from the updated PGD [3].

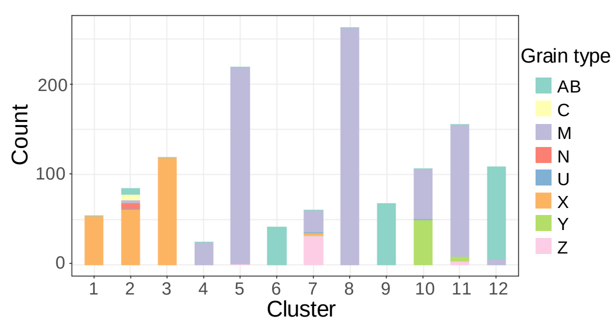

Fig. 2: Histogram showing the resulting clusters, compared with previously assigned grain types shown with colors [2-3].

Our cluster analysis suggests the presence of 12 different clusters for SiC presolar grains (Fig. 2), which are compared with the previous classification. Overall, derived clusters are in agreement with previously defined SiC groups but also highlight several discrepancies between our model output and previous classification. For instance, AB grains form three different clusters (clusters 6, 9, and 12), having different ranges of $^{14}N/^{15}N$, and including a cluster of grains (6) with relatively low $^{14}N/^{15}N$, $\delta^{29}Si$, and $\delta^{30}Si$ (Fig. 3). In addition, the maximum $^{14}N/^{15}N$ value for this cluster 6 is close to the solar ratio, which coincides with a recently proposed division between AB1 and AB2 grains having sub- and super-solar N isotopic ratios respectively [5]. Our clustering suggests however, another division for AB2 grains which should be assessed in future studies by comparing them with astrophysical models.

X grains form three different clusters including one (cluster 3) with Si isotopic compositions lying along a line intersecting the solar composition and with a slope of ~2/3, similar to the subgroup X1 identified by [6]. In addition, cluster 2 includes several grains having a Si isotopic composition close to the subgroup X2 [6], with additional C, N, U, and a few mainstream (M) and AB grains (Fig. 2). Finally, cluster 1 contains grains with large excesses in ^{28}Si and do not correspond with any of the previously defined subgroups of X grains.

Y grains, which were defined as having a $^{12}C/^{13}C$ ratio higher than 100, are found clustered with some M grains (10). Z grains are also clustered with some M grains (7). Finally, a majority of M grains are included in four clusters: cluster 4 having solar C, N, and Si isotopic compositions, clusters 8 and 5 with homogeneous $^{12}C/^{13}C$ ratios close to 50 and 70, respectively, and cluster 11 having heterogeneous N and C isotopic compositions and slightly more excesses in ^{30}Si than other clusters.

Conclusions and outlook: Our preliminary results suggest a larger number of SiC groups than the original classification (12 instead of 8) with the division of the three main groups M, X, and AB into different clusters. Additional cluster analysis, including data on other isotopic compositions such as those of Ti and Al, will be presented at the meeting.

References: [1] Zinner E. K. (2014) *Treatise on Geochemistry*, 2nd ed., Elsevier, 181–213. [2] Hynes K. M. and Gyngard F. (2009) *LPS 40*, Abstract #1198. [3] Stephan T. et al. (2020) *LPS 51, this meeting*. [4] Hazen R. (2019) *Am. Min., 104*, 810-816. [5] Liu N. et al. (2017) *ApJL, 842*, L1. [6] Lin Y. et al. (2002) *ApJL 575*, 257–263.

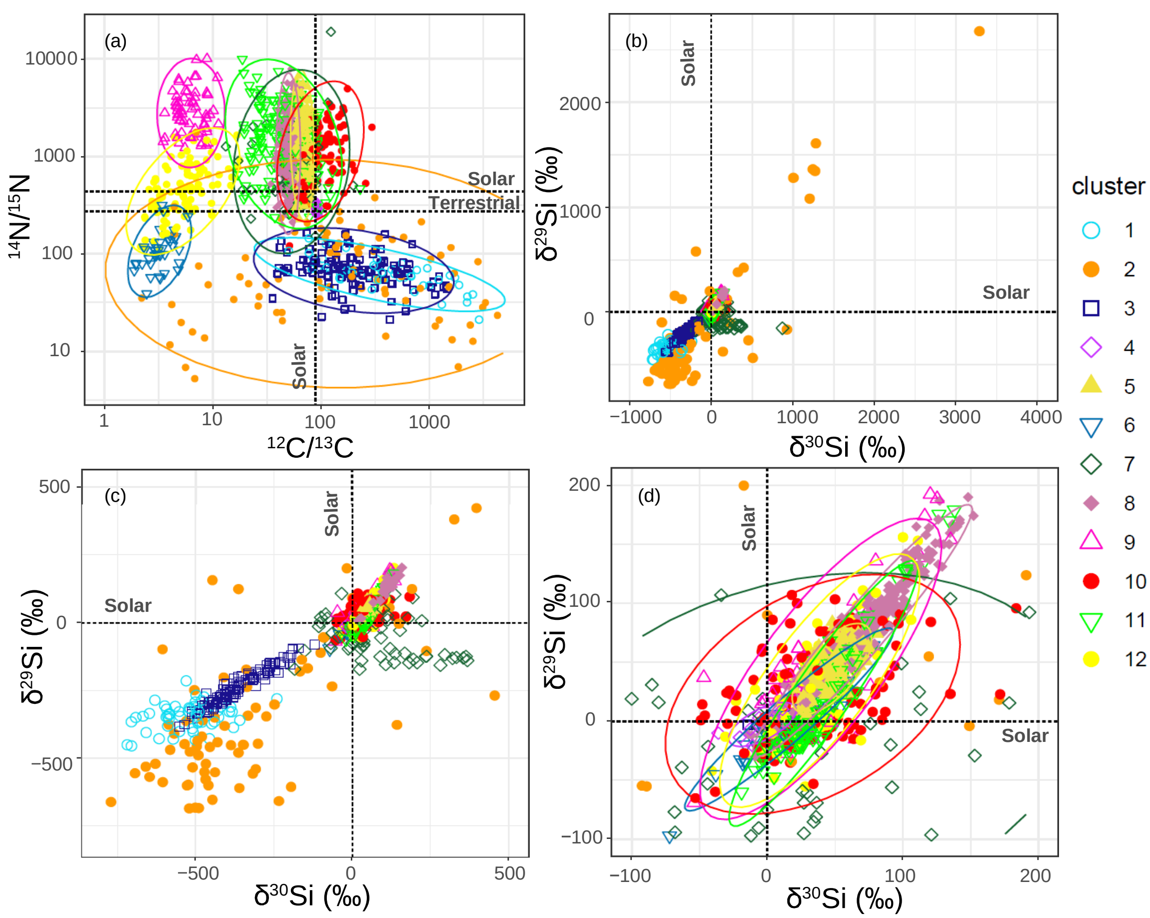

Fig. 3: (a) $^{14}N/^{15}N$ versus $^{12}C/^{13}C$ and (b-d) $\delta^{29}Si$ versus $\delta^{30}Si$ for SiC presolar grains [4]. Resulting clusters from our cluster analysis are shown with different symbols. (c) and (d) are zoomed diagrams of (b).