From ancient minerals to new materials: Melting temperature prediction using a graph neural network model

August 29 2022

Credit: Pixabay/CC0 Public Domain

If you apply enough heat, at some point, most things melt, just like ice cream on a hot summer day.

Knowing exact melting temperatures is critical for building any high-performance material. The building and safety of bridges, gas turbines, jet engines and heat shields on aircraft are dependent on knowing the performance limits of materials. Materials are often synthesized or processed employing the molten or liquid state, so knowing melting is critical to making new materials.

Shift to the field of Earth and planetary science, and the melting points are used to reveal clues into Earth's past and the characteristics of planets in our solar system and far-out orbiting exoplanets.

But measuring the melting temperature of a compound or material is an arduous task. That's why, of the estimated 200,000-plus inorganic compounds, less than 10% of their melting temperatures are known.

Melting temperatures are often measured after carefully calibrating crystal structures or plotting the thermodynamic free energy curves when a material melts, creating a phase change from a solid to a liquid. This is analogous to the melting of solid ice to form liquid water. But when high-temperature materials exceed 2,000 or 3,000 degrees, finding an experimental chamber to do the measurements can be a challenge. And sometimes, rocks have complex mixtures of minerals not much larger than a grain of sand—so getting enough sample of a single mineral can also present a challenge. Materials synthesized under extreme conditions of high pressure and temperature are also often available in only very small amounts.

Now, Arizona State University researchers Qi-Jun Hong, Alexandra Navrotsky, and Sergey Ushakov, together with Axel van de Walle at Brown University have harnessed the power of artificial intelligence (AI), or machine learning (ML), to demonstrate an easier way to predict melting temperatures for potentially any compound or chemical formula.

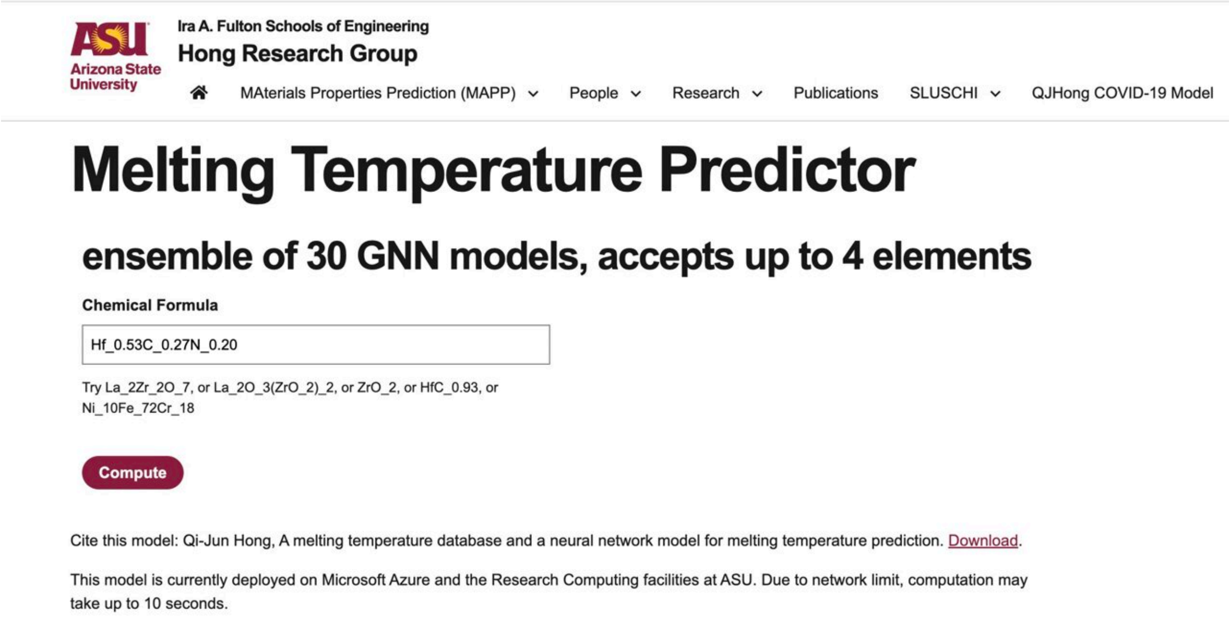
"We employ machine learning methods to fill this gap by building a rapid and accurate mapping from chemical formula to melting temperature," said Hong, assistant professor in the School for Engineering of Matter, Transport and Energy, within the Ira A. Fulton Schools of Engineering.

"The model we have developed will facilitate large-scale data analysis involving melting temperature in a wide range of areas. These include the discovery of new high-temperature materials, the design of novel extractive metallurgy processes, the modeling of mineral formation, the evolution of Earth over geological time, and the prediction of exoplanet structure."

Hong's approach allows melting temperatures to be computed in milliseconds for any compound or chemical formula input. To do so, the research team built a model from an architecture of neural networks, and trained their machine learning program on a custom-curated database encompassing 9,375 materials, out of which 982 compounds have melting temperatures higher than a scorching 3100 degrees Fahrenheit (or 2000 degrees Kelvin). Materials at this temperature glow white-hot.

Hong used this methodology to explore two lines of research: 1) predicting the melting temperatures of nearly 5,000 minerals and 2) finding new materials that have extremely high melting temperatures above 3000 Kelvin (or 5000 degrees Fahrenheit).

For the minerals project, Hong's team was able to predict melting temperatures and correlate these with the known major geological epochs of Earth's history. These AI-garnered melting temperatures were applied to minerals made since the formation of Earth about 4.5 billion years ago. The oldest minerals originate directly from stars or interstellar and solar nebula condensates predating Earth's formation 4.5 billion years ago. These are the most refractory, with melting temperatures around 2600 F.



Melting Temperature Predictor

ensemble of 30 GNN models, accepts up to 4 elements

Chemical Formula: Hf_0.53C_0.27N_0.20

Try La_2Zr_2O_7, or La_2O_3(ZrO_2)_2, or ZrO_2, or HfC_0.93, or Ni_10Fe_72Cr_18

Cite this model: Qi-Jun Hong, A melting temperature database and a neural network model for melting temperature prediction. Download.

This model is currently deployed on Microsoft Azure and the Research Computing facilities at ASU. Due to network limit, computation may take up to 10 seconds.

The team made their model simple and reliable enough so that any user can obtain the melting temperature within seconds for any compound based only on its chemical formula. Credit: Qijun Hong, Arizona State University

For the most part, there was a gradual decrease in the calculated melting temperatures of minerals identified on Earth with more recent time, with two major exceptions.

"The gradual overall decrease in the melting temperature of minerals formed during Earth history is interrupted with two anomalies, which are distinctly pronounced in average and medium melting temperatures using 250 or 500 million years ago binning," said Navrotsky, an ASU Professor with joint faculty appointments in the School of Molecular Sciences and School for Engineering of Matter, Transport and Energy and Director of MOTU, the Navrotsky Eyring Center for Materials of the Universe.

The first anomaly in Earth's early history came from a dramatic temperature spike caused by a scary and dynamic time of major meteor strikes, including the possible formation of the Moon.

"The spike at 3.750 billion years ago correlates to the proposed timing of late-heavy bombardment, hypothesized exclusively from dating of lunar samples and currently debated," said Navrotsky.

The team also noticed a large temperature dip in the melting temperatures of minerals around 1.75 billion years ago.

"The dip at 1.750 billion years ago is related to the first known occurrences of a large number of hydrous (water-containing) minerals and correlates with the Huronian glaciation, the longest ice age thought to be the first time Earth was completely covered in ice."

With their machine learning program trained to successfully replicate mineral melting in Earth's early history, next, the team turned their attention to finding new materials that have extremely high melting temperatures. Dozens of new materials are identified and computationally predicted to have extremely high melting temperatures above 5,000 degrees Fahrenheit (3000 Kelvin), more than half the temperature of the Sun's surface.

The team made their model simple and reliable enough so that any user can obtain the melting temperature within seconds for any compound based only on its chemical formula.

"To use the model, a user needs to visit the webpage and input the chemical compositions of the material of interest," said Hong. "The model will respond with a predicted melting temperature in seconds, as well as the actual melting temperatures of the nearest neighbors (i.e., the most similar materials) in the database. Thus, this model serves as not only a predictive model, but a handbook of melting temperature as well."

The model, hosted by ASU's Research Computing Facilities, is now publicly available at the ASU webpage: https://faculty.engineering.asu.edu/hong/melting-temperature-predictor/.

The research was published in the *Proceedings of the National Academy of Sciences*.

More information: Melting temperature prediction using a graph neural network model: From ancient minerals to new materials, *Proceedings of the National Academy of Sciences* (2022). DOI: 10.1073/pnas.2209630119

Provided by Arizona State University

Citation: From ancient minerals to new materials: Melting temperature prediction using a graph neural network model (2022, August 29) retrieved 26 June 2024 from https://phys.org/news/2022-08-ancient-minerals-materials-temperature-graph.html

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