Specific Heat Prediction on Web

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Introduction

A web application has been developed to predict specific heat as a dependence of temperature base on chemical formulas of compounds, using machine learning method and Neumann Koop's law. The Debye temperature can also be calculated by fitting the specific heat curve to Debye model.

Table 1 Machine learning method

Algorithm	Random Forest
Evaluation method	10-fold Cross Validation
Target variable	Specific heat
Descriptor	Atomic number Atomic mass Temperature

Neumann Koop's law:

$$C = \sum_{i=1}^{n} (C_i \cdot f_i)$$

C_i and f_i denote the specific heat and mass fraction of the *i-th* constituent

Specific Heat Prediction

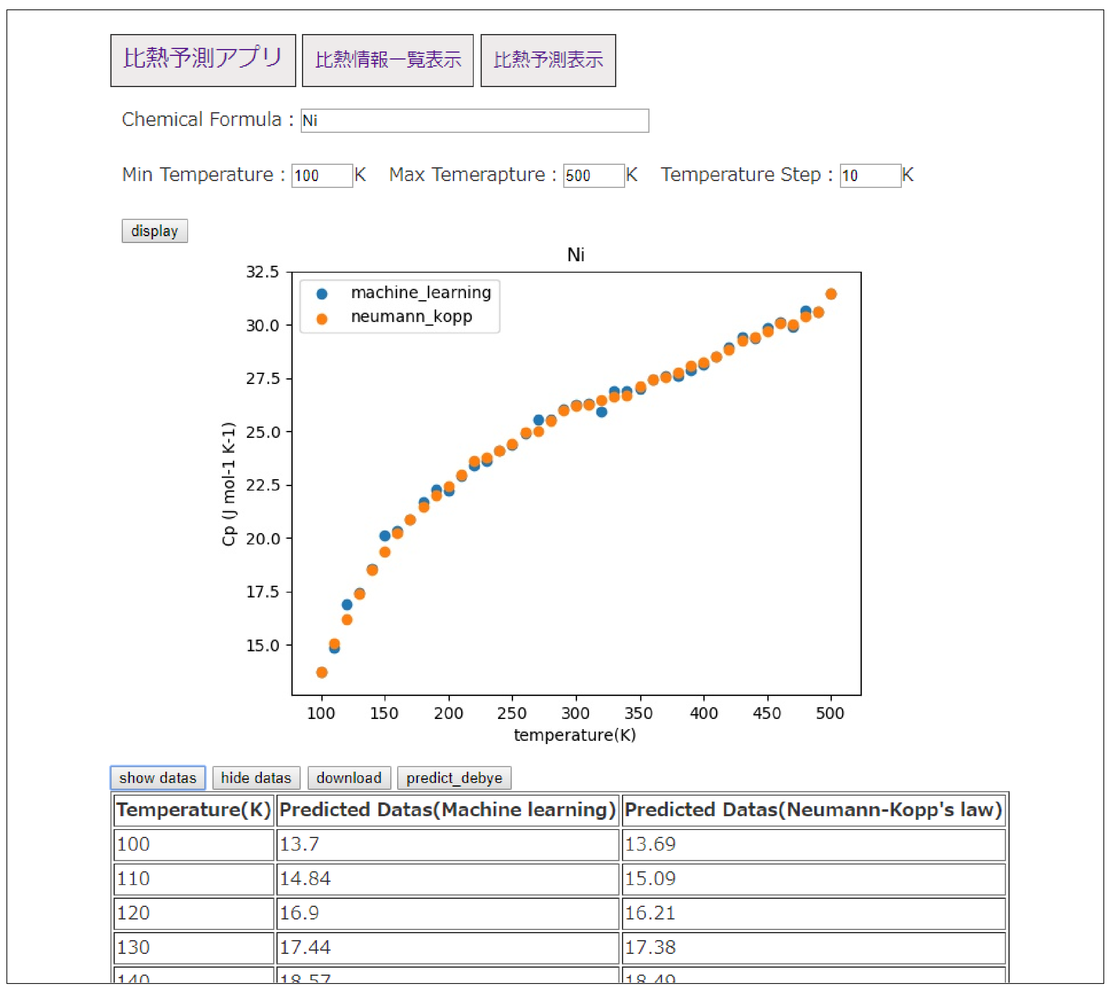

Fig. 1 Plot of predicted specific heat as a function of temperature. The data is also available as tabular format and can be downloaded as a csv file.

We have evaluated multiple machine learning algorithms (Fig. 2), and adopted the "Random forest" being used in the web application.

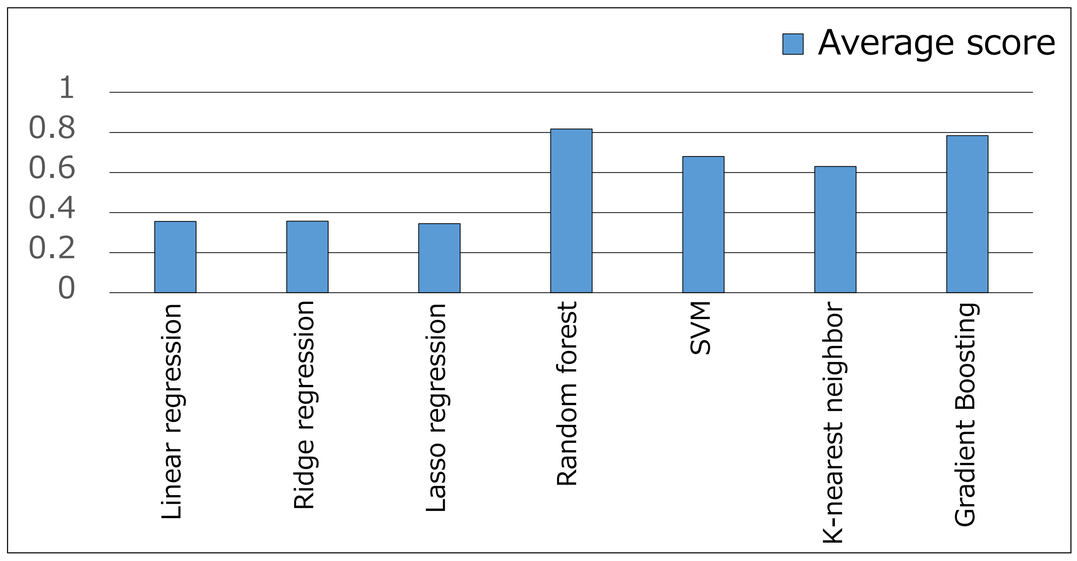

Fig. 2 Algorithm evaluation result

Fitting of Debye temperature

Debye temperature can be calculated by fitting the specific heat curve to Debye model at a temperature range below Debye temperature, and the whole Debye specific heat curve is show to compare with the experimental values.

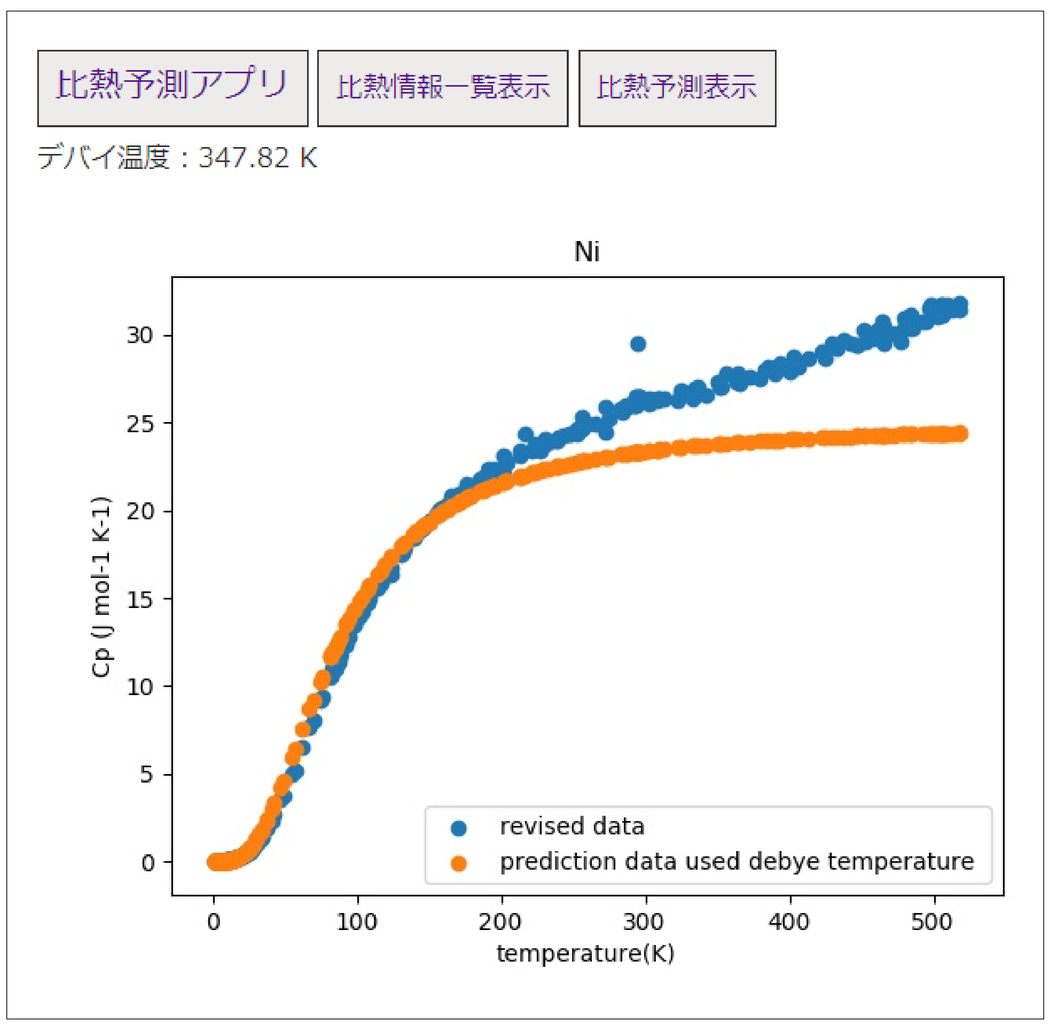

Fig. 3 Fitting of Debye temperature and comparison of Debye specific heat curve with experimental values.