Predicting high-Tc Transmon candidates with minimal Oxide Thickness

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Abstract

The current coherence time record of 0.3 milliseconds in superconducting Tantalum remains insufficient for most problems. A recent discovery by McLellan and Dutta et. al [1] demonstrated 1/3rd of qubit decoherence was attributable to oxide layers grown on the material surface. Based on this information, this project focused on the creation and expansion of metrics that quantify the desirability of a material based on its predicted oxide amounts and predicted critical temperature. The gradient boosting algorithm XG Boost was used for predictive models, and the Nelder-Mead optimization algorithm was used to solve the Convex Hull minimization problem posed when calculating energetically favorable oxide amounts.

Calculated Metrics

The noise introduced by oxide layers might be avoided by selecting superconducting materials that do not form oxides, or form thermally removable oxides. To quantify these options, the following were calculated.

A. Oxidation Metric *How energetically favorable is oxide formation?*

For a given material Q, say we have *n* possible oxides and *m* elements in its elemental formula. We can create the following matrices / vectors.

- **Matrix M,** *n by m*: From the *n* possible oxides, find how much of each *m* elements they contain. Combine these coefficients into **M** such that each row contains the amount of element found in the oxides.
- **Vector E,** *n by 1*: Contains the respective formation energy of oxides
- **Vector C,** *m by 1:* Contains the ordered amount of Q's elements in each oxide from the parsed formula.
- **Vector A,** *n by 1:* Target vector with amounts of each oxide. Will be optimized, but initial guess is $\mathbf{M^T \cdot C}$.

These inputs can then be input into a Nelder-Mead optimization, discussed further in methods. The final metric is then:

$$\Delta H_{Material} = QForm_{ation\ Energy} \qquad \Delta H_{Oxides} = \sum A \cdot E \quad \text{(Net Energy)}$$

$$\boldsymbol{Metric} = 1 - \frac{\Delta H_{Oxides} - \Delta H_{Material}}{\Delta H_{Oxides}}$$

B. % Meltable Oxide *How much of the oxide is thermally removable?*

The melting temperature of each oxide can be found through ASU Hong Group's Melting Temperature prediction API. Finding the optimized mass of each oxide from part **A**, we get:

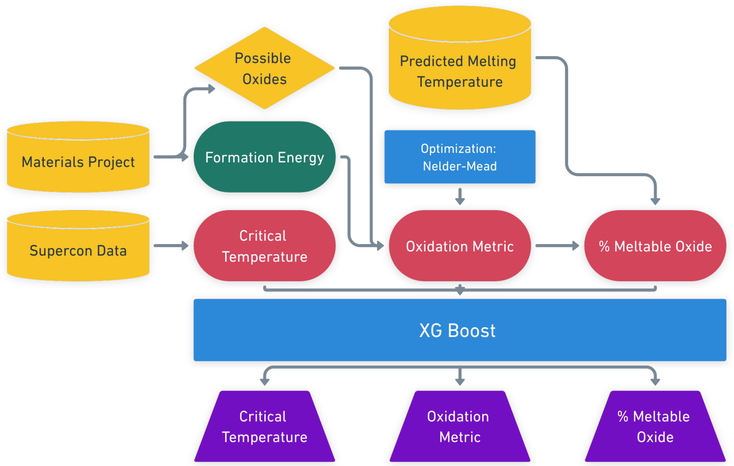
$$\boldsymbol{Melted\ Oxide}\ \% = \frac{\boldsymbol{Mass\ of\ meltable\ oxides}}{\boldsymbol{Net\ mass\ of\ oxides}}$$

C. Critical Temperature (Tc) *When is our material superconductive?*

In general, higher critical temperatures correlate to higher qubit coherence times – See Methods for prediction algorithm.

Optimization Methods

This project used data from the Materials Project and the Supercon database.



For the Nelder-Mead optimization during the Oxidation Metric calculation, a maximum iteration of 100000 was imposed for computational limitations. Constraints to preserve the conservation and positivity of mass were implemented by multiplying our loss function (The total energy of the oxides, or A · E) by a simple exponential function penalizing constraint breaches.

After obtaining initial calculations for the Oxidation Metric and Critical Temperature, these metrics were extended to all materials on our dataset using a predictive model based on the XG-Boost algorithm. Input data was formed based on the elemental composition of each material, and elemental information was weighted according to the parsed chemical formula. Settings for the XG Boost algorithm were as follows:

Evaluation Metric: RMSE, Max Depth: 16, Minimum Weight: 1, Learning rate: 0.02, Boosting rounds: 375.

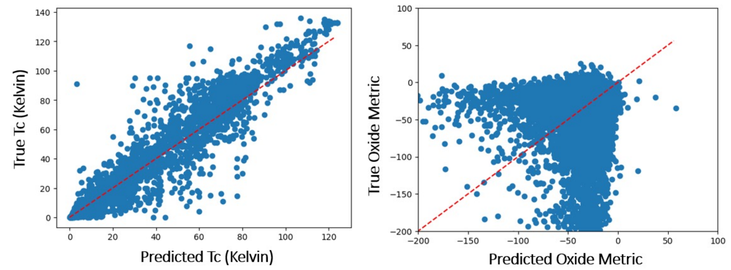
Discussion

While using machine learning methods to predict material properties, it is important to consider the inherent limitations of these methods. As seen in the poor predictions of the Oxidation Metric, input data may not be enough to capture the complexity of certain features. Additionally, undiscovered relations between materials, such as those necessary for room-temperature superconductivity, may not be contained within data collected thus far due to the lack of discovered room-temperature superconductors to begin with.

For future usage of these metrics, the code necessary to quickly build these models is available on github: https://github.com/nsong03

Results

Due to the low number of boosting rounds and limited tree complexity used with the XG Boost algorithm, overfitting to our large dataset for these results is highly unlikely. Expanding on Hamidieh's work [3], we found that the critical temperature of materials could be accurately predicted using machine learning methods solely from elemental data. However, our calculated oxide metric was not so predictable.



It was found that the critical temperature of materials in the SuperCon dataset could be predicted with an RMSE of ~9.4, with a significant portion of error contributions coming from repeated entries within the SuperCon dataset itself.

For the Oxidation Metric however, accurate predictions were not made with our optimization algorithm. A consistent RMSE of > 40 was observed, regardless of boosting rounds or tree complexity. This implied that the input elemental composition information was not enough to form statistically meaningful connections between materials and our calculated Oxidation Metric. A simpler oxidation metric was tested with only the single most likely oxide used for calculations; This yielded an RMSE of < 9.

Conclusions

This work has developed a collection of metrics to analyze materials on a large scale. By locating materials grouped within a close Cartesian distance to each other (within the context of our three metrics), clusters with similar superconducting properties can be identified. As the materials project is inclusive of many theoretical materials, this provides valuable initial insights into which candidates may be useful for high Tc, high coherence time superconductors. Additional products such as the solution to the Convex Hull problem provide initial estimates for oxide layer thicknesses. It remains an open, important question of why exactly oxide layers promote qubit decoherence. Initial ideas point towards the two-level systems created by dangling electrons in the oxide layers, noise created by rough interfaces, or external microwave / phonon vibrations amplified in between the oxide layers. To approach this goal, simulations are currently underway on Tantalum oxidation.

References

[1] 'Chemical profiles of the oxides on tantalum in state of the art superconducting circuits', McLellan and Dutta et. al., Jan 2023
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[3] 'A Data-Driven Statistical Model for Predicting the Critical Temperature of a Superconductor', Hamidieh 2018