SC-CoMIcs: A Superconductivity Corpus for Materials Informatics

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Abstract
This paper describes a novel corpus tailored for the text mining of superconducting materials in Materials Informatics (MI), named SuperConductivity Corpus for Materials Informatics (SC-CoMIcs). Different from biomedical informatics, there exist very few corpora targeting Materials Science and Engineering (MSE). Especially, there is no sizable corpus which can be used to assist the search of superconducting materials. A team of materials scientists and natural language processing experts jointly designed the annotation and constructed a corpus consisting of manually-annotated 1,000 MSE abstracts related to superconductivity. We conducted experiments on the corpus with a neural Named Entity Recognition (NER) tool. The experimental results show that NER performance over the corpus is around 77% in terms of micro-F1, which is comparable to human annotator agreement rates. Using the trained NER model, we automatically annotated 9,000 abstracts and created a term retrieval tool based on the term similarity. This tool can find superconductivity terms relevant to a query term within a specified Named Entity category, which demonstrates the power of our SC-CoMIcs, efficiently providing knowledge for Materials Informatics applications from rapidly expanding publications.

Keywords: Materials Informatics, Superconductivity Corpus, Named Entity Recognition, Materials Text Mining

1. Introduction
Recently, Materials Informatics (MI) is a hot topic in the field of Material Science and Engineering (MSE). The reason behind this surge of interests is that a lot of materials scientists are trying to use machine learning to accelerate the search of new materials. To find new materials, scientists need to select base materials, adequate doping, and process conditions to synthesize the materials. This is a very costly, time-consuming process. Traditionally, the experience and intuition of researchers often led to unexpected discovery of new useful materials. MI is studied with great expectation to change the paradigm in such a long process of materials discovery. There has been, however, a bottleneck, i.e., existence of few datasets for MI to work effectively [Ramprasad et al., 2017].

The search of superconducting materials is one of the most challenging issues in MSE. Even after historical discovery of high-Tc cuprate superconductors [Bednorz and Müller, 1986], materials with a higher transition temperature, higher current flow, and higher processability are required for practical applications [Malozenoff et al., 2005; Foltyn et al., 2007]. In materials exploration, experts often consult thousands of published and new articles for getting knowledge to decide a research direction. This can be one of the factors that hinder the efficient search of superconducting materials. In this paper, we propose a new corpus named SuperConductivity Corpus for Materials Informatics (SC-CoMIcs) tailored for the superconductivity domain, evaluate the corpus using state-of-the-art Natural Language Processing (NLP), and introduce a term search tool which efficiently provides knowledge hidden in a large amount of literature. To this end, we here particularly focus on construction of Named Entity Recognition (NER) model based on manually-annotated corpus, which categorizes entities useful for materials scientists and thus provides new ideas in the search of new superconducting materials.

2. Annotation Design
A team of materials scientists and natural language processing experts jointly designed annotations. Term categories are carefully considered to match the requirements from the domain experts. As a preparation for annotations, we initially referred to a keyword list of letter journal *scripta materialia*, and the domain experts updated it for enrichment. The original keyword list has five categories: Synthesis/Processing, Characterization, Material Type, Property/Phenomena, and Theory/Computer Simulation/Modeling. We modified this categorization and defined the following seven categories as summarized in Table 1.

Characterization: The Characterization category lists the terms of characterization methods such as X-ray diffraction (XRD) and scanning electron microscope (SEM). The information is useful in MSE in relation to Element and Property.

Process: The Process category lists the terms of Synthesis/Processing such as the sol-gel method for film samples, calcination for bulk samples, and AC/DC sputtering for thin-film preparation. This information is hardly obtained from theoretical simulations such as density functional theory, thus providing unique database useful for materials scientists.

Property: The Property category lists the terms of Property/Phenomena and their Theoretical representations such as electrical conductivity, mechanical hardness, electron-phonon coupling, and Fermi surface. Property and Theory including Simulation and Modeling can belong to each different category. In this work, we unified them into the Property category because they are sometimes difficult to be distinguished.

1https://www.elsevier.com/__data/promis/misc/SMM%20Keywords.pdf
### 3. Corpus Construction Workflow

This section explains the corpus creation workflow from data collection to annotation steps.

We conducted two-round annotation processes. The first round was conducted as a trial annotation since there was no annotations that we can referred to when we started this annotation in 2018. We collected 200 abstracts and manually annotated them. In the second round, we collected 800 abstracts and then conducted pattern matching-based automatic annotation using a term list for each category. We finally manually annotated terms in the 800 abstracts.

In the remainder of this section, we explain document collection, pattern matching, and manual annotation.

### 3.1. Document Collection

We collected abstracts through ScienceDirect Web API from February to June in 2019. In the first round, we first selected about 4,000 abstracts, issued from 1983 to 2018, with the query “supercond*” and finally selected 200 abstracts that include:

- at least one superconductivity term,
- at least one term which means doping or transition temperature,
- more than or equal to 100 words.

In the second round, we were more confident about abstract selection based on the experience in the first round and selected about 11,000 abstracts, issued from 2010 to 2019, by the query “superconductivity”. Then we finally selected 800 abstracts that are not included in the 200 first round abstracts and include:

- at least one term for each of superconductivity, doping, element/compound,
- more than or equal 100 words.

### 3.2. Automatic Labeling by Pattern Matching

We then conducted pattern matching-based automatic annotation using a term list for each category compiled from the annotated corpus and the keyword list enriched by experts in addition to the original list of *scripta materialia*. This pattern matching-based annotation step was included to alleviate the manual annotation burden.

In the pattern matching of term lists against abstracts, we basically performed matching within generated variations of term list entries. Specifically, we applied lemmatization process and regular expression based pattern matching. In the lemmatization process, we removed entry inflections.

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**Table 1: Term categories**

| Category          | Explanation                      | Example               |
|-------------------|----------------------------------|-----------------------|
| Characterization  | characterization methods          | X-ray diffraction, SEM|
| Process           | synthesis and process            | sol-gel, calcination, sputtering |
| Property          | materials properties             | electrical, cryogenic, magnetic fields |
| Material          | structural entities, sample descriptors | tetragonal, P4/nmm, bulk, film, grain |
| Element           | elements, compounds              | Ti, oxygen, YBa$_2$Cu$_3$O$_7$ |
| Doping            | doping operation                  | doping, addition, doped |
| Value             | quantitative information with units | 100K, 5-10µm |

**Figure 1: Annotation sample**

**Material:** The Material category lists the terms of structural entities and sample descriptors such as tetragonal crystal symmetry, bulk/film sample, and grain boundary. The information augments the details of the sample whose composition is defined by Element.

**Element:** The Element category lists names and symbols of elements and compounds such as Ti, oxygen, and YBa$_2$Cu$_3$O$_7$ or YBCO. This is strictly distinguishable from the Material category as entities in the Element category can be expressed by chemical composition formulae.

**Doping:** Since the doping often changes materials properties significantly, we added the Doping category to represent doping operations such as doping, substitute, and addition.

**Value:** The Value category targets numerical values with units, such as 160K. This enables to extract transition temperatures and process conditions, for example.

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6754
such as “ing” and “ed”. By combining a lemma word and suffixes such as “ing” or “ed” with OR operator by using regular expression, we extend the coverage of their word forms. Note that this process targets for term labels other than Element and Value. This is because Element can take various kinds of compound names and Value can have a different value each time.

3.3. Manual Annotation

The first round was performed by a well-experienced domain expert and the second round was conducted by four annotators, who are undergraduate and master students in material science or relevant areas according to the annotation guideline created during the first round annotation. We used BRAT (Stenetorp et al., 2012) annotation tool, which is a browser-based annotation environment for collaborative text annotation. After the first and second rounds, we corrected minor errors while checking the data formats, such as dual labeling of the same terms. This is because when a term has two category labels, training and testing of NER are interfered. At the same time, when a term had different categories in a different appearance, we left this dual labels as contextual difference. Figure 1 shows an example of completed annotations that is visualized with BRAT.

4. Corpus Analysis

This section explains corpus statistics and annotator agreement results.

4.1. Corpus Statistics

Table 2 shows statistics of the SC-CoMics corpus. Terms in the Material, Property and Element categories appear a lot in the corpus. The Doping and Value categories also appear sufficient number times; the latter is beneficial to extract quantitative information from text in relation to superconductivity terms. The number of Characterization terms is relatively small; however, the frequency of Characterization terms per se is not a problem as described in Section 5.3. Figures 2 and 3 show the histograms of the numbers of sentences per abstract and tokens per sentence. Most abstracts contain round 4-8 sentences and most sentences have around 20-35 words.

4.2. Annotator Agreements

For the second round, we evaluated annotator agreement. We asked the four annotators to annotate extra 10 abstracts independently, without telling that they were annotating the same 10 abstracts. The domain expert, who annotated in the first round, also created reference annotations for the 10 abstracts.

The annotation scores were calculated based on the both exact-span and label match. Table 3 shows the agreement between each annotator and the domain expert. Annotator A performed slightly better than others, although there is no significant difference in the total scores. On the other hand, there are some variations in the agreement rates by categories. Characterization and Doping have high agreement rates. Material and Property have relatively low agreement rates of around 70% because these are difficult or ambiguous for annotation, e.g., “anisotropic” and “order”; the annotator needs to consider contexts based on the domain knowledge to judge the annotation.

We also calculated the Fleiss’ kappa to measure the agreement between the four annotators, which is independent of expert annotation. This is a token level evaluation based on the BIO labels and it takes into account all pairs of four annotators. As a result, we obtained the Fleiss’ kappa score of 83.1%.

After the independent annotation by the four annotators in the second round, all the annotations of 800 abstracts were reviewed by four annotators. This implies that the resulting
Table 3: Agreement scores of four annotator’s (A, B, C, and D) annotations with respect to the reference annotations

| Category     | Annotator A | Precision | Recall | F1     | Annotator B | Precision | Recall | F1     |
|--------------|-------------|-----------|--------|--------|-------------|-----------|--------|--------|
| Characterization | 0.947       | 0.900     | 0.923  | 0.905  | 0.950       | 0.927     |
| Material     | 0.867       | 0.697     | 0.773  | 0.771  | 0.607       | 0.679     |
| Property     | 0.817       | 0.744     | 0.779  | 0.774  | 0.774       | 0.774     |
| Element      | 0.964       | 0.951     | 0.957  | 0.837  | 0.796       | 0.816     |
| Doping       | 1.000       | 1.000     | 1.000  | 0.974  | 0.884       | 0.927     |
| Process      | 0.933       | 0.824     | 0.875  | 0.906  | 0.853       | 0.879     |
| Value        | 0.730       | 0.836     | 0.780  | 0.750  | 0.927       | 0.829     |
| Total (micro-ave.) | 0.879     | 0.822     | 0.850  | 0.812  | 0.777       | 0.794     |

| Category     | Annotator C | Precision | Recall | F1     | Annotator D | Precision | Recall | F1     |
|--------------|-------------|-----------|--------|--------|-------------|-----------|--------|--------|
| Characterization | 0.727       | 0.800     | 0.762  | 0.900  | 0.900       | 0.900     |
| Material     | 0.779       | 0.607     | 0.682  | 0.911  | 0.754       | 0.825     |
| Property     | 0.703       | 0.732     | 0.717  | 0.757  | 0.649       | 0.699     |
| Element      | 0.818       | 0.761     | 0.788  | 0.815  | 0.838       | 0.826     |
| Doping       | 0.966       | 0.651     | 0.778  | 0.969  | 0.721       | 0.827     |
| Process      | 0.735       | 0.735     | 0.735  | 0.788  | 0.765       | 0.776     |
| Value        | 0.776       | 0.945     | 0.852  | 0.688  | 0.800       | 0.739     |
| Total (micro-ave.) | 0.769     | 0.729     | 0.749  | 0.813  | 0.752       | 0.781     |

The corpus would have better annotation quality than the agreement rates in Table 3

5. Experiments

5.1. Experimental Settings

Recently, Bidirectional Encoder Representations from Transformers (BERT) (Devlin et al., 2018) is used in various NLP applications and contributed to improve performance. We used the pre-trained embedding model SciBERT (Beltagy et al., 2019), which is a BERT model that is trained on a large-scale scientific literature. BERT is a contextual embedding model, which means that an embedding vector of the same word changes according to the surrounding words. We used the SciBERT NER model with the default parameter settings, which is provided along with the SciBERT model.

The input for SciBERT NER was the SciBERT (uncased) pre-trained model. SciBERT NER is a stack of Bi-LSTM→CRF layers and determines category labels in the form of IOB2 tagging. In the preprocessing, we removed inner NE annotations in the nested annotations.

5.2. NER Performance

We evaluated the NER performance using the 10-fold cross validation. In the training, SciBERT embedding models were fixed, i.e., no fine tuning applied. The evaluation results are shown in Table 4. The scores in the table are the averages of ten times of training. Compared to the human annotator agreement rates, the NER achieved quite comparable performance to most of the human annotators. Table 5 shows results for each fold of the cross validation.

5.3. Learning Curves

To see whether the number of training data is sufficient or not, we draw learning curves by changing the number of training data from 100 to 900 by the 100 unit. We trained each model ten times and computed the average of the scores. The results are displayed in Figure 4. The scores grow as the number of data increases. When we used 900 abstracts, the recognition performance of Doping, Characterization, and Property seems to be saturated but that of Process and the other categories are still slightly increasing. The number of occurrences of Characterization terms in the corpus is relatively small; however, since its NER performance seems to be saturated using 900 training abstracts, the number of Characterization terms in the corpus is not a serious problem; while its NER performance has room to improve as its human annotator performance is mostly much higher. We believe that we need to use domain knowledge to improve the recognition performance of Characterization terms. In general, the size of the SC-CoMics corpus is proved to be mostly sufficient while the larger data is the better for some categories, same as the cases in any machine learning-based approaches.

5.4. Applications with Word Similarity

To see the usefulness of our corpus, we created a term retrieval tool (Figure 5) based on the word similarity using word2vec (Mikolov et al., 2013). We used the word2vec module in the gensim (Reháček and Sojka, 2010) Python library. The used algorithm is the skip-gram with negative sampling. The details of the parameter settings are shown in Table 6. While BERT and its family are contextual embedding models and need a large amount of corpus, word2vec is more suitable for generating word vectors from annotated 10,000 abstracts.
| Category    | Precision | Recall | F1   |
|-------------|-----------|--------|------|
| Characterization | 0.780    | 0.771  | 0.774 |
| Material    | 0.752    | 0.738  | 0.743 |
| Property    | 0.734    | 0.689  | 0.711 |
| Element     | 0.842    | 0.869  | 0.855 |
| Doping      | **0.960** | **0.964** | **0.961** |
| Process     | 0.739    | 0.729  | 0.733 |
| Value       | 0.807    | 0.635  | 0.709 |
| **Total (micro-ave.)** | **0.784** | **0.754** | **0.768** |

Table 4: Scores of SciBERT NER

| Fold | Precision | Recall | F1   |
|------|-----------|--------|------|
| 1    | 0.793     | 0.752  | 0.772 |
| 2    | 0.706     | 0.714  | 0.710 |
| 3    | 0.721     | 0.754  | 0.737 |
| 4    | 0.788     | 0.756  | 0.772 |
| 5    | 0.809     | **0.778** | 0.793 |
| 6    | 0.806     | 0.751  | 0.778 |
| 7    | 0.786     | 0.734  | 0.759 |
| 8    | 0.809     | 0.757  | 0.782 |
| 9    | 0.817     | **0.778** | **0.797** |
| 10   | 0.809     | 0.761  | 0.784 |

Table 5: Scores for each fold: * indicates the fold in which the first annotated 200 abstracts are used as a test data for SciBERT NER tool.

Every multi-word NE term is converted into a single token except for the Element term that consists of a list of compound names, which represents a main target superconducting material entity of the abstract. In the present study, we separated Element terms, which include more than one element, into pieces. For example, an Element term “YBa$_2$Cu$_3$O$_7$” is separated into “Y”, “Ba”, “Cu”, “O”. This simple conversion of compound names is useful to capture distances among elements based on existing compounds and the related entities through embedding.

We automatically annotated 9,000 abstracts using the NER model trained over our corpus. Using the corpus and automatically annotated abstracts, we created word vectors with the 300 dimensionality by the gensim word2vec tool. The term retrieval tool finds terms relevant to the query term using the trained word2vec word vectors. The special feature of this tool is that we can specify categories to show as relevant terms. Table 7 shows the ranked retrieval results of queries “film” and “bulk” in the Process category. Note that, abbreviations are removed from the ranked terms. The terms with * are those which are judged by experts reasonably to be categorized in Process. The most of the terms are correctly categorized, legitimating the present NER model; except a few errors such as field-cooled and liquid nitrogen temperature which seem to be in Process but should be conditions of Characterization. The entities selected with “film” query include overall typical processing for film samples; those selected with “bulk” query include reasonably the bulk processing. These Process entities can be further selected by combining another query, for example, a compound name. In contrast, without annotated documents, we cannot focus on a specific category of terms as shown in Table 8, where we find few terms categorized in Process.

### 6. Related Work

There are plenty of NER datasets which target general English documents, mostly news articles. The CoNLL 2003 dataset (Sang and De Meulder, 2003) have four named entity tags: LOC (location), ORG (organization), PER (person) and MISC (miscellaneous). Ontonotes 5.0 (Pradhan et al., 2013) handles wider range of documents including phone conversations and Web pages. In the biomedical area, there are a lot of annotated corpus, such as the GENIA corpus (Kim et al., 2003). In the chemistry area, CHEMDNER (Krallinger et al., 2015) targets extraction of chemical materials with seven fine grained categories, such as abbreviations and identifiers. i2b2 challenge 2010 data (Uzuner et al., 2011) targets the extraction of medical concepts from radiology reports.

On the other hand, there are few manually annotated corpora in Materials Science and Engineering. Exceptions are matscholar (Weston et al., 2019), the materials synthesis corpus (Mysore et al., 2019), and (Foppiano et al., 2019). The matscholar has annotations of seven entities, such as material names, synthesis methods, and applications. However, it targets the general material science domain while we focus on superconducting domain. In addition, we include numerical expressions, such as temperatures, which are essential for finding new superconductors. For reference, inter-annotator agreement of this corpus was 87.4%. The materials synthesis corpus is annotated information re-
lated to the synthesis process, such as operations and their typed arguments. In this work, quantitative information is handled as part of typed arguments. However, because it targets only the paragraphs of the synthesis process, the resultant corpus is different from ours and not suitable for the purpose of this study, where we deal with a wide range of corpus related to superconductivity. For reference, its inter-annotator agreements were 20.5-97.1%, which highly depend on the categories. (Foppiano et al., 2019) studies an information extraction task on superconducting materials domain, whose direction is close to our work. They annotated material names and transition temperatures on five full papers, and obtained pair sets of these entities. However, our experimental results showed that we need the amount of around 1,000 annotated abstracts to obtain mostly stable results.

There are a few studies that worked on information extraction using the material science corpora. (Tamari et al., 2019) proposed a method for generating action graphs from material process texts in the framework of reinforcement learning by using the material synthesis corpus. (Onishi et al., 2018) proposed distant supervised learning framework to extract relationships with a small number of annotated texts. Based on the extracted relationships, a process-structure-property-performance (PSPP) design chart (Olson, 2013) was constructed.

Our sizable annotated corpus focuses on comprehensive knowledge of superconductivity described in 1,000 abstracts.

### 7. Conclusions and Future Work

In this paper, we constructed a novel manually-annotated corpus, SC-CoMiCs, tailored for extracting information related to superconductivity. This corpus is essential for extracting not only material names and process information but also doping and quantitative information. Around 75-85% of annotator agreements is similar to those of other corpora (Weston et al., 2019; Mysore et al., 2019) in MI. We also performed experiments of SciBERT NER on the corpus, and achieved the F1-scores of approximately 77%, which is comparable to the human annotator agreements. The learning curves also support that the size of the corpus is mostly sufficient enough. Our future work includes using the NER results in downstream applications such as relation extraction and summarization, and constructing term as well as document retrieval systems, which would support discovery of new superconducting materials.

| rank | word                  | score     |
|------|-----------------------|-----------|
| 1    | ISD                   | 0.45202   |
| 2    | epitaxially           | 0.43835   |
| 3    | epitaxially grown     | 0.40697   |
| 4    | substrate temperature | 0.40086   |
| 5    | ion beam              | 0.39507   |
| 6    | epitaxial growth      | 0.39161   |
| 7    | deposited             | 0.39049   |
| 8    | partial melting       | 0.38841   |
| 9    | depositions           | 0.38562   |
| 10   | Growth                | 0.38024   |

Figure 5: demo page
| Rank | Term                        | Similarity | Term                        | Similarity |
|------|-----------------------------|------------|-----------------------------|------------|
| 1    | *epitaxially                | 0.4384     | *melt-processed             | 0.3608     |
| 2    | *epitaxially grown          | 0.4070     | *sintered                   | 0.3018     |
| 3    | *substrate temperature      | 0.4009     | *milled                     | 0.2905     |
| 4    | *ion beam                   | 0.3951     | *welded                     | 0.2762     |
| 5    | *epitaxial growth           | 0.3916     | *Growth                     | 0.2760     |
| 6    | *deposited                  | 0.3905     | *pressed                    | 0.2729     |
| 7    | *partial melting            | 0.3884     | *infiltration               | 0.2678     |
| 8    | *depositions                | 0.3856     | *ex-situ                    | 0.2659     |
| 9    | *Growth                     | 0.3802     | *heat treatment temperature | 0.2599     |
| 10   | *reactive sputtering        | 0.3785     | *sintering temperatures     | 0.2598     |
| 11   | *growth parameters          | 0.3779     | *joined                     | 0.2586     |
| 12   | *deposition                 | 0.3757     | *ball-milled                | 0.2580     |
| 13   | *seeding                    | 0.3747     | *powder-in-tube method      | 0.2576     |
| 14   | *pyrolysis                  | 0.3692     | *solidified                 | 0.2570     |
| 15   | *heat treatment temperature | 0.3684     | *solid-state reactions      | 0.2555     |
| 16   | *melt-processed             | 0.3682     | field-cooled                | 0.2531     |
| 17   | *sputtering pressure        | 0.3678     | liquid nitrogen temperature | 0.2517     |
| 18   | *dc sputtering              | 0.3656     | *partial melting            | 0.2512     |
| 19   | *growth temperature         | 0.3647     | field-cooling               | 0.2415     |
| 20   | *as-deposited               | 0.3635     | *melt growth                | 0.2385     |

Table 7: Term retrieval results with Process category restriction.

| Rank | Term                        | Similarity | Term                        | Similarity |
|------|-----------------------------|------------|-----------------------------|------------|
| 1    | films                       | 0.5081     | magnetized                 | 0.3870     |
| 2    | crack-free                  | 0.4472     | single-domain              | 0.3738     |
| 3    | *epitaxially                | 0.4384     | iron-arsenide              | 0.3683     |
| 4    | magnetic shield             | 0.4339     | Bulk                       | 0.3644     |
| 5    | buffered                    | 0.4270     | *melt-processed            | 0.3608     |
| 6    | film surface                | 0.4264     | single-grain               | 0.3591     |
| 7    | c-axis orientation          | 0.4230     | single grains              | 0.3552     |
| 8    | buffer layers               | 0.4170     | levitation force            | 0.3537     |
| 9    | substrate                   | 0.4150     | *levitation                | 0.3513     |
| 10   | sapphire                    | 0.4122     | guidance force             | 0.3497     |
| 11   | Flat                        | 0.4112     | permanent magnet guideway  | 0.3463     |
| 12   | domain structure            | 0.4108     | single domain              | 0.3424     |
| 13   | substrate surface           | 0.4104     | high-T c superconductor    | 0.3318     |
| 14   | buffer layer                | 0.4072     | bulk magnet                | 0.3241     |
| 15   | *epitaxially grown          | 0.4070     | pellet                      | 0.3200     |
| 16   | nanodots                    | 0.4066     | magnetic stiffness          | 0.3198     |
| 17   | faceted                     | 0.4021     | critical current anisotropy | 0.3196     |
| 18   | *substrate temperature      | 0.4009     | bulks                       | 0.3195     |
| 19   | surface roughness           | 0.3992     | type II superconductor     | 0.3144     |
| 20   | *ion beam                   | 0.3951     | joint resistance            | 0.3100     |

Table 8: Term retrieval results without Process category restriction.
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