QuenchMiner^{TM}: Decision Support for Optimization of Heat Treating Processes *

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Abstract. This paper describes a Decision Support System (DSS) for the heat treating of materials built using artificial intelligence. Heat treating encompasses the controlled heating and cooling of materials to achieve desired properties. Data gathered during heat treating is a source of knowledge useful in making decisions. This knowledge discovered through data mining is used to build a DSS that helps materials scientists conduct studies to improve heat treating processes. The data is also used to draw graphs based on which material microstructures can be predicted. A major challenge here is accurately estimating microstructures at different points on a graph under varying conditions of interest. Another big challenge is simulating expert judgment while mining over simple and complex data types, by incorporating domain-specific facts in the mining process. Our work is one of the first to integrate knowledge discovery and data visualization into one system for supporting materials science processes.

Keywords. Data Mining, Knowledge Discovery, Visualization, Heat Treating, Decision Support.

1 Introduction

Areas of artificial intelligence have applications in several domains, providing motivation for further research. The work described in this paper is an example of such an application. It is a Decision Support System (DSS) [1] called QuenchMiner^{TM} built with the goal of optimizing the processes in heat treating, using data mining [2] and data visualization [3] techniques.

Application Domain. *Heat Treating* is a field in *Materials Science* [4]. It involves the controlled heating and cooling of metals and other materials to achieve specific mechanical and thermal properties. *Quenching*, i.e., rapid cooling, is an important step in the heat treating operations [5]. The setup used for quenching [6] at the Center for Heat Treating Excellence (CHTE), at WPI is shown in Figure 1. The material being quenched is called the part, probe or workpiece. The cooling medium is called the quenchant.

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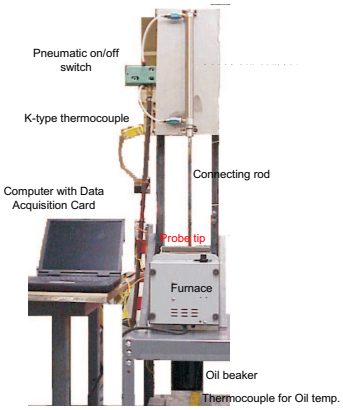

Fig. 1. CHTE Quenching Setup

Motivation. Data obtained from quenching experiments is a source of knowledge useful in making decisions. For instance, if experimental observations indicate that, *"Excessive agitation of the quenchant implies greater distortion of the part"*, then this rule could be used to computationally estimate distortion when agitation is known. This assists in making decisions about selecting quenching conditions for optimal performance. This is an example of rule-based data mining [2] for decision support [1]. There are also decisions based on graphs and charts. For example, a material has different microstructural characteristics at different points on a *cooling curve* [5] [1]. These influence its properties, which in turn affect decisions about selection of materials. The ability to visualize microstructures at various regions on a graph is thus important. The need to mine and visualize data and use this to support decision making serves as motivation for QuenchMiner^{TM}.

Challenges. The visualization of microstructure under *different* quenching conditions is a challenging task. This augments state-of-the-art techniques, and is being addressed in our research. Another challenge is predicting cooling curves and related curves obtained from quenching experiments, in addition to estimating parameters such as distortion. This is being addressed in our ongoing research on graph-based data mining.

2 Decision Support in Heat Treating

A *Decision Support System* is defined as a system in which one or more computers and computer programs assist in decision making by providing information [1]. QuenchMiner^{TM} provides decision support in heat treating by achieving the following goals.

[1] A cooling curve is the graph of temperature versus time plotted during a quenching experiment, whose slopes at different points give the cooling rates.

Parameter Estimation. The system estimates parameters of interest such as cooling rate and distortion tendency [5] given the quenching input conditions, without performing the experiment. This supports decisions about the selection of quenchants, parts and quenching conditions in the industry to achieve a desired output.

Microstructure Prediction. It also predicts and visualizes microstructure at different points along a cooling curve [5]. Since the microstructure determines properties such as hardness, its prediction assists in making decisions about selecting materials for specific processes.

2.1 Design of System

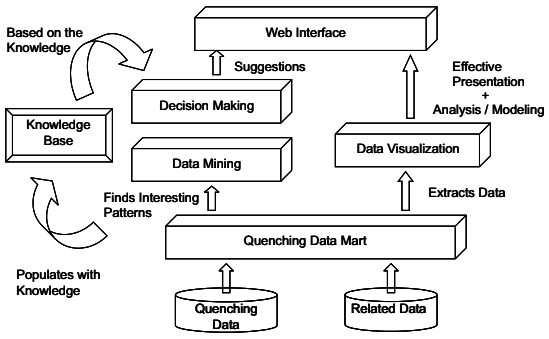

Fig. 2. QuenchMiner^{TM} Architecture

The DSS is designed using the architecture shown in Figure 2. The quenching data such as experimental details, and related data such as literature, are integrated into a quenching data mart [7]. A *Data Mart* is a repository of data gathered from operational and other sources, designed to serve a particular community of knowledge workers [8]. In this case, the focus is on the heat treating community.

The data mining component discovers knowledge using the data in the quenching data mart. The knowledge, mainly rules representing tendencies, populates the knowledge base, forming domain expertise in heat treating. The decision making unit has the logic of an inference engine in an *Expert System* [9] [2]. In other words, this unit has the ability to reason using the rules in the knowledge base.

The data visualization component extracts quenching data and models it for effective presentation. This primarily focuses on estimating the microstructure of the part during various stages of quenching, thereby helping users to understand the behavior of the part.

The users interact with the system through a web interface. This enables worldwide access to the authorized users of QuenchMiner^{TM}.

[2] An Expert System is a computer program that represents and reasons with knowledge of some specialist subject with a view to solving problems or giving advice.

3 Data Mining and Knowledge Discovery

Data Mining [2] is the process of discovering interesting patterns and trends in large data sets for guiding future decisions. Data mining thus leads to the discovery of knowledge from raw data. Many people treat data mining as a synonym for a popularly used term *Knowledge Discovery in Databases or KDD.* After studying a variety of data mining techniques in detail, it was determined that the most relevant to mining numeric and character data from quenching experiments is *Association Analysis* [10].

3.1 Association Analysis

Association Analysis is the discovery of *Association Rules* [10] showing attribute-value conditions that occur frequently together in a given set of data. For example, the results of several experiments may indicate that if the quenchant has low viscosity and if the agitation velocity in the setup is high, then the part cools faster. This is converted into an association rule as follows.

Low Viscosity ^ Excessive Agitation-Velocity => Fast Cooling-Rate

Rules such as this are useful for decision support in QuenchMiner^{TM}. The *Apriori algorithm* [10] has been used for association analysis of heat treating data. This is based on the *Apriori property* which states that, *"All nonempty subsets of a frequent itemset must also be frequent"* [10]. This is used to prune infrequent itemsets by eliminating their infrequent subsets while mining over data. Frequent itemsets are likely to lead to rules.

Metrics called *confidence* and *support* are used to determine the significance of the rules. These are defined based on probability of occurrence [2,10].

Confidence(A=>B) = P(B | A) : probability of B given that A occurs.

Support(A=>B) = P(A U B) : probability of A and B across all itemsets.

These measures are used to define priorities for rules. Priorities indicate the relative importance of rules in decision making.

3.2 Challenges in Data Mining

Estimating cooling curves and other related curves, in addition to predicting parameters such as cooling rate, is an issue of interest to users. This involves mining over graphs and charts and is more challenging than mining over numeric and character data. This is part of our ongoing research and is being addressed through domain-type-dependent data mining over complex data types, in this case, graphs obtained from quenching experiments.

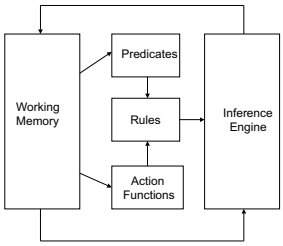

Fig. 3. Decision Making Unit

4 Analysis using Discovered Knowledge

The system architecture of the decision making unit is shown in Figure 3. This uses rule interpreters. A *Rule Interpreter* is a subsystem that is designed to apply a given set of rules to perform analysis and make decisions [9].

Forward Chaining. The rule interpreter technology used here is forward chaining. *Forward Chaining* is a method that finds every conclusion possible based on a given set of premises, [9,11]. In this approach, inference rules are applied to knowledge, leading to new assertions. This process repeats forever until some stopping criterion is met. The system stores the facts in a memory called the working memory, in our context, the facts being the quenching input conditions. The rules are stored in a knowledge base. In each cycle, the system computes the subset of rules whose left hand side is satisfied by the current contents of the working memory. Certain left hand side conditions may be treated as *predicates* [3]. The system then decides which of these rules should be executed. The final step in each cycle is to execute the actions, represented in the action functions, on the chosen rules.

Rete. A technique called *Rete* [11] is used to match the rules to the facts. The rete match algorithm is an efficient method for comparing a large collection of patterns to a large collection of objects. [11]. Rete compiles the memory into a network that eliminates duplication over time. It ensures that the same rule is not executed on the same arguments twice. It also ensures that in case of conflicts, it executes the rule with the highest priority [9]. Thus, rete improves the efficiency and accuracy of the decision making process.

The logic of the decision making unit in QuenchMiner^{TM} is outlined in the algorithm and example below.

```
FOR y = 1 to m STEP 1
        Iy.value = user-entry /* list of input variables */
FOR x = 1 to n STEP 1
        Ox.name = user-select /* list of output parameters */
FOR x = 1 to n STEP 1 /* iterate through each o/p param. */
        v1 = 0, v2 = 0 /* initialize variables for tendencies */
        FOR y = 1 to m STEP 1
                IF Ox := Iy THEN /* if o/p param. depends on i/p var. */
                        IF Iy.value => v1 /* v1 is one extreme of tendency */
                        THEN v1 = v1 + wgt1 /* wgt1 is extent of impact */
```

[3] Predicates are properties of objects or relations between objects that can be used as logical representations of conditions, e.g. "viscosity-low" is a predicate.

```
                        ELSE IF Iy.value => v2 /* other extreme */
                                THEN v2 = v2 + wgt2 /* update var. by weight */
                NEXT y
                IF v1 > v2 /* check which tendency is greater */
                THEN final-tendency = v1
                ELSE IF v1 < v2
                        THEN final-tendency = v2
                        ELSE final-tendency = avg(v1, v2) /* balance of extremes */
                Ox.value = final-tendency /* determine final tendency */
        NEXT x
        FOR x = 1 to n STEP 1 /* for each o/p param. */
                OUTPUT Ox.value /* convey tendency to user */
```

Algorithm: QuenchMiner^{TM} Decision Making Unit

```
FOR y = 1 to 3 STEP 1 /* list of input variables */
        quenchantCategory = water, partGeometry = cylinder, partSurface = smooth
FOR x = 1 to 1 STEP 1 /* list of output parameters */
        coolingUniformity = yes /* parameter of interest */
FOR x=1 /* coolingUniformity */
        v1(uniform) = 0, v2(nonUniform) = 0 /* initialize tendency variables */
        coolingUniformity depends on quenchantCategory, partGeometry, partSurface.
                quenchantCategory = water => v2 = 0 + 4 = 4 /* update nonUniform */
                partGeometry = cylinder => v1 = 0 + 4 = 4 /* update uniform */
                partSurface = smooth => v1 = 4 + 2 = 6 /* update uniform */
        v1 > v2 /* since v1 = 6 and v2 = 4 */
        final-tendency = v1 /* represents uniform cooling */
NEXT parameter /* no more parameters */
OUTPUT coolingUniformity = uniform /* convey this to user */
```

Example: Estimation of Cooling Uniformity

5 Visualization of Microstructure

Data Visualization is a technique to present a set of data in the form of graphical depictions [12,13]. The goals of visualization include comparing sets of data, indicating directions and the locations of actions or phenomena, relating values and concepts, and revealing the features of the data.

A *microstructure* is what one sees when an alloy specimen is cut, its surface polished and etched to expose phases, and put under a microscope [4]. Predicting microstructures of the alloys interests materials scientists and engineers because microstructures dictate mechanical properties such as hardness, toughness, and ductility.

5.1 Methodology for Visualization

The architecture of the visualization component is illustrated in Figure 4. Java servlets and JSP provide the API between the database server and the web interface, and the mapping of the data to the visualization primitives. Communication with users occurs through a web interface, with Java applets to provide data sharing at minimum cost and maximum ease of use.

The volume fractions of what phases are present in the resulting microstructure can be determined by tracing what regions the time-temperature curve goes through and for how long. As the cooling progresses, new phases start to form along different regions of the curve, and grains grow at the same time. The

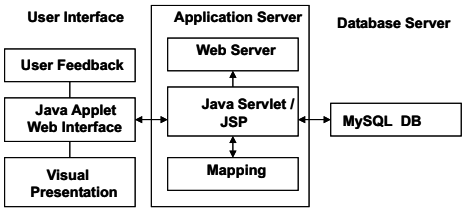

Fig. 4. Visualization Component

changes in volume fractions in the material during the cooling process can be represented in two ways, a line graph and a pie chart, as shown in Figures 5 and 6 respectively. Here A and B represent the fractions.

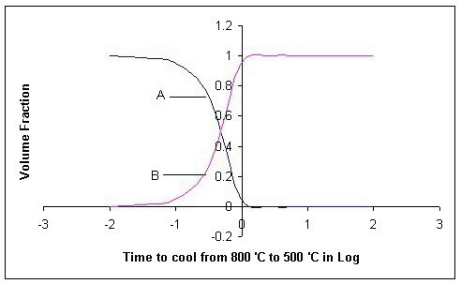

Fig. 5. Line Graph of Volume Fractions

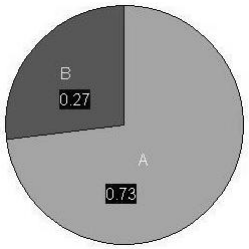

Fig. 6. Pie Chart of Volume Fractions

5.2 CCT Diagrams and Time-Temperature Data

Continuous cooling transformation diagrams and time-temperature curves are the two elements used in microstructure predictions. The *Continuous Cooling Transformation* or CCT diagram of an alloy shows when and at what temperature the phase transitions start and end [5]. The chemical composition of the alloy is the major deciding factor here. An example of a CCT diagram for a $0.4\%C$, $1.5\%Mn$, $0.5\%Mo$ steel is shown in Figure 7 [14]. The labels austenite, ferrite, bainite, and pearlite are the names of steel phases. The evolution of the microstructures resulting from quenching can be modeled by superimposing these time-temperature curves from the experiment over the CCT diagram for the alloy as shown.

5.3 Challenges in Visualization:

Time-temperature data taken at *various locations* of quenched specimens from several experiments are available from the database. This separates this project from existing tools, as we aim to predict microstructures under *different* quenching conditions of interest, as opposed to existing techniques.

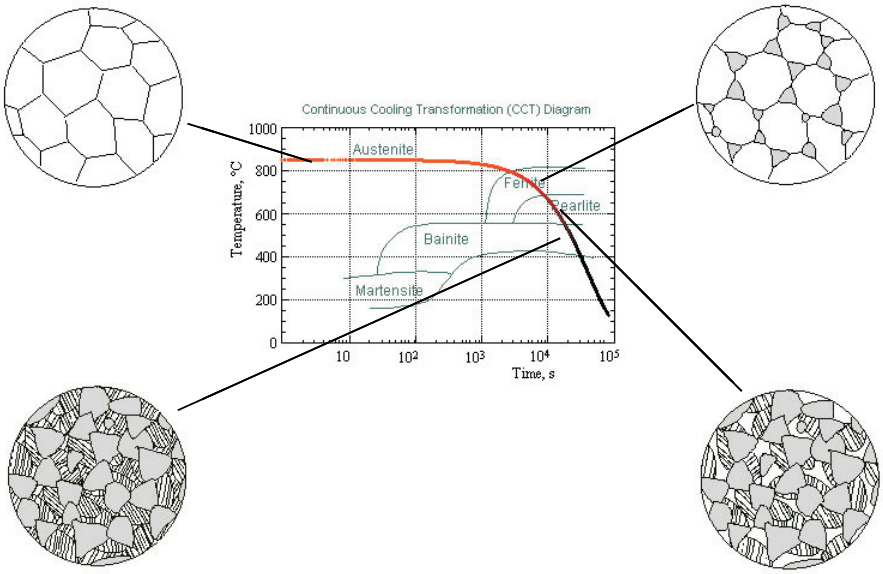

Fig. 7. CCT Diagram and Predicted Microstructures

6 Performance Evaluation

DSS Experiments. An example from the evaluation of QuenchMiner^{TM} is presented here. In this example, the DSS is asked to estimate the average heat transfer coefficient [15] [4], given the quenching conditions. Figure 8 shows the user input for this case and Figure 9 shows the output estimated by the DSS. The system estimates that under the given conditions, the average heat transfer coefficient is likely to be on the higher side. The time taken by the system for processing is approximately 1 second.

Comparison with Quenching Experiments. The same input conditions as in the above example are used to run a quenching experiment, and curves are plotted from its results, as shown in Figures 10 and 11. On studying these, a heat treating expert would infer that, in this experiment, the average heat transfer coefficient is on the higher side. The time taken for all this is totally about 1 hour. The resulting estimation is similar to the DSS estimation.

Hence, QuenchMiner^{TM} provides a quick and reasonably accurate estimate of the parameters of interest. Similar experiments have been performed on the visualization component. From the experiments, the users have inferred that QuenchMiner^{TM} serves as an effective DSS in the heat treating domain, achieving an acceptable level of efficiency and accuracy. Further improvements are in progress.

[4] The heat transfer coefficient represents the heat extraction capacity in quenching as determined by part density, quenchant temperature and other factors.

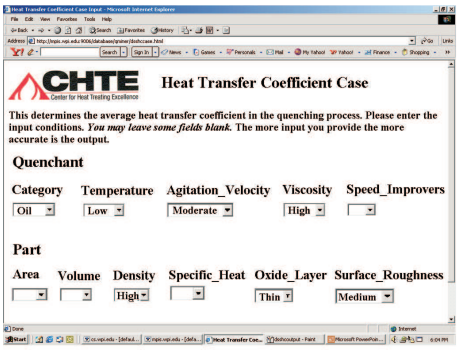

Fig. 8. User Input

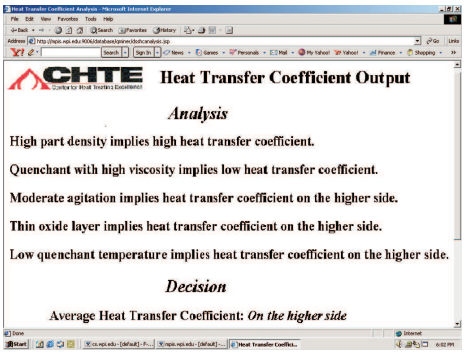

Fig. 9. DSS Output

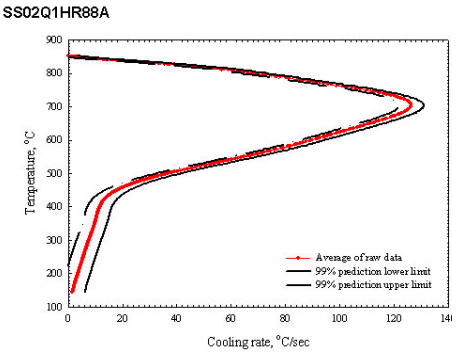

Fig. 10. Cooling Rate Curve

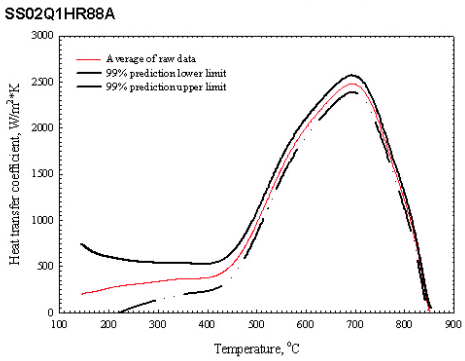

Fig. 11. Heat Transfer Curve

7 Related Work

Our earlier work in this area includes QuenchPAD^{TM} [6], the Quenchant Performance Analysis Database, developed for storage and querying of quenching data. QuenchMiner^{TM}, in addition to storage and retrieval, provides decision support. Materials databases such as EQUIST [16], data mining systems such as WEKA [17] and data visualization systems such as XMDV [3] have been developed. However, to the best of our knowledge, QuenchMiner^{TM} is novel, being an integration of *Knowledge Discovery* and *Data Visualization* for *Decision Support* in the *Heat Treating of Materials*.

8 Conclusions

Data mining and visualization techniques have been applied to the heat treating domain to build a Decision Support System called QuenchMiner^{TM}. This assists heat treating users, enabling them to retrieve data at a glance and use it to assist

decision making for optimizing processes. It sets the stage for further research in data mining and visualization as needed to address certain challenges. Rigorous evaluation of the system is in progress for further enhancement.

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