Material data extraction from journal articles using large language models

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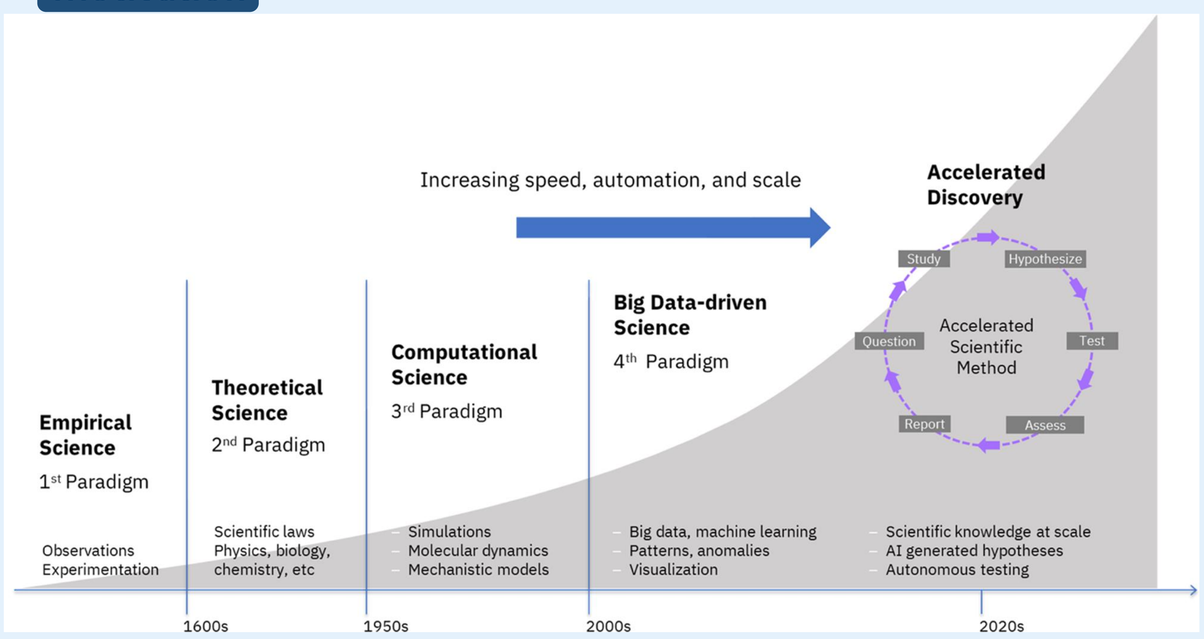
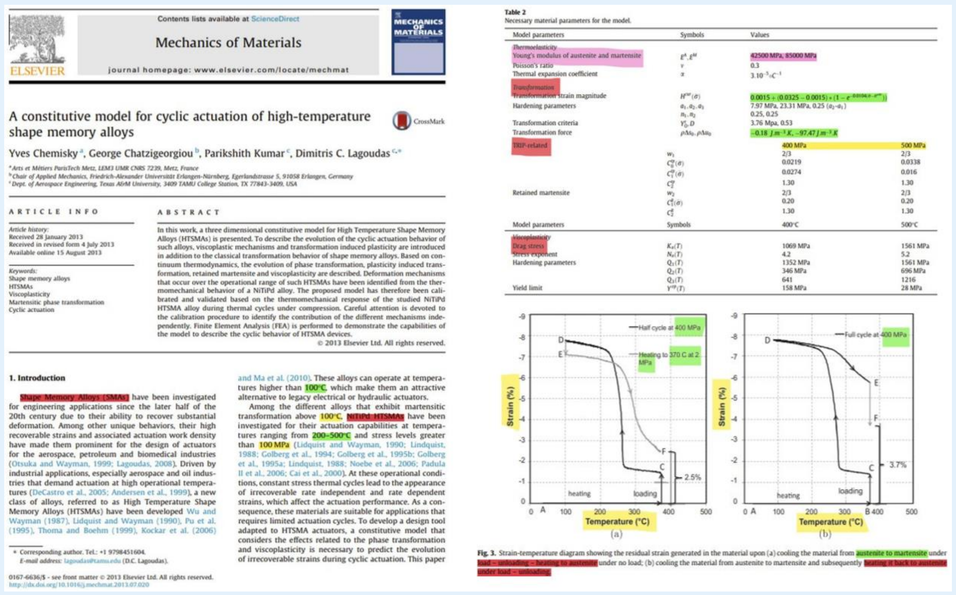
Objectives

- To establish a framework to extract materials' data in a structured format from research sinks.
- To test the framework on a sub-field in materials science and evaluate the performance of the framework when used with different LLMs.

Motivation





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A constitutive model for cyclic actuation of high-temperature shape memory alloys

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ABSTRACT

In this work, a three dimensional constitutive model for High Temperature Shape Memory Alloys (HTSMAs) is presented. To describe the evolution of the cyclic actuation behavior of such alloys, viscoplastic mechanisms and transformation induced plasticity are introduced in addition to the classical transformation behavior of shape memory alloys. Based on continuum thermodynamics, the evolution of phase transformation, plasticity induced transformation, retained martensite and viscoplasticity are described. Deformation mechanisms that occur over the operational range of such HTSMAs have been identified from the thermomechanical behavior of a NiTiPd alloy. The proposed model has therefore been calibrated and validated based on the thermomechanical response of the studied NiTiPd HTSMA alloy during thermal cycles under compression. Careful attention is devoted to the calibration procedure to identify the contribution of the different mechanisms independently. Finite Element Analysis (FEA) is performed to demonstrate the capabilities of the model to describe the cyclic behavior of HTSMA devices.

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1. Introduction

Shape Memory Alloys (SMAs) have been investigated for engineering applications since the later half of the 20th century due to their ability to recover substantial deformation. Among other unique behaviors, their high recoverable strains and associated actuation work density have made them prominent for the design of actuators for the aerospace, petroleum and biomedical industries (Otsuka and Wayman, 1999; Lagoudas, 2008). Driven by industrial applications, especially aerospace and oil industries that demand actuation at high operational temperatures (DeCastro et al., 2005; Andersen et al., 1999), a new class of alloys, referred to as High Temperature Shape Memory Alloys (HTSMAs) have been developed Wu and Wayman (1987), Lidquist and Wayman (1990), Pu et al. (1995), Thoma and Boehm (1999), Kockar et al. (2006) and Ma et al. (2010). These alloys can operate at temperatures higher than 100 °C, which make them an attractive alternative to legacy electrical or hydraulic actuators.

Among the different alloys that exhibit martensitic transformation above 100 °C, NiTiPd-HTSMAs have been investigated for their actuation capabilities at temperatures ranging from 200–500 °C and stress levels greater than 100 MPa (Lidquist and Wayman, 1990; Lindquist, 1988; Golberg et al., 1994; Golberg et al., 1995b; Golberg et al., 1995a; Lindquist, 1988; Noebe et al., 2006; Padula II et al., 2006; Cai et al., 2008). At these operational conditions, constant stress thermal cycles lead to the appearance of irrecoverable rate independent and rate dependent strains, which affect the actuation performance. As a consequence, these materials are suitable for applications that requires limited actuation cycles. To develop a design tool adapted to HTSMA actuators, a constitutive model that considers the effects related to the phase transformation and viscoplasticity is necessary to predict the evolution of irrecoverable strains during cyclic actuation. This paper

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Table 2
Necessary material parameters for the model.

Model parameters	Symbols	Values
Thermoelasticity		
Young's modulus of austenite and martensite	E^A, E^M	42500 MPa, 85000 MPa
Poisson's ratio	ν	0.3
Thermal expansion coefficient	α	$3.10^{-6}.C^{-1}$
Transformation		
Transformation strain magnitude	$H^{sat}(\sigma)$	$0.0015 + -0.0125 \ldots 0.0015(1 - e^{-8.95(\sigma + \ldots)})$
Hardening parameters	a_1, a_2, a_3	7.97 MPa, 23.31 MPa, 0.25 ($a_3 = a_2$)
	n_1, n_2	0.25, 0.25
Transformation criteria	Y_0^t, D	3.76 Mpa, 0.53
Transformation force	$\rho\Delta s_0, \rho\Delta h_0$	$-0.18\ J.m^{-3}.K, -97.47\ J.m^{-3}$
TRIP-related		400 MPa / 500 MPa
	w_1	2/3 / 2/3
	$C_1^a(\sigma)$	0.0219 / 0.0338
	$C_1^m(\sigma)$	0.0274 / 0.016
	C_1^a	1.30 / 1.30
Retained martensite	w_2	2/3 / 2/3
	$C_2^a(\sigma)$	0.20 / 0.20
	C_2^a	1.30 / 1.30
Model parameters	Symbols	400°C / 500°C
Viscoplasticity		
Drag stress	$K_0(T)$	1069 MPa / 1561 MPa
Stress exponent	$N_0(T)$	4.2 / 5.2
Hardening parameters	$Q_1(T)$	1352 MPa / 1561 MPa
	$Q_2(T)$	346 MPa / 696 MPa
	$Q_3(T)$	641 / 1216
Yield limit	$Y^M(T)$	158 MPa / 28 MPa

Fig. 3. Strain-temperature diagram showing the residual strain generated in the material upon (a) cooling the material from austenite to martensite under load → unloading → heating to austenite under no load; (b) cooling the material from austenite to martensite and subsequently heating it back to austenite under load → unloading.

Materials Data in academic works

Methods

0. **Data Collection:**
Elsevier API+ XML Parsing of research articles to obtain the different sections of the paper.

1. **Prompt Engineering:**
Prompts: Context + few shot examples+ formatting instructions+ article

Context:

1. An alloy is a solid mixture of multiple elements. Its chemical composition conveys the amount of each element present in the alloy. For example, an alloy with chemical composition AlCoCr contains elements Al, Co and Cr in equal amount. Similarly, an alloy with chemical composition $Al_2Co_3Ni_5$ contains 2 parts Al, 2 parts Co and 5 parts Ni.
2. Here are some of the common structures adopted by alloys

…

n. Abbreviations for subsequent thermo-mechanical processes are: CR=Cold Rolled; FC=Furnace Cooled; FOR=Forged; HIP=Hot Isostatic Pressing; HPT=High Pressure Torsion; HR=Hot Rolled; VHP=Vacuum Hot Pressed; WQ=Water Quenched

Few shot examples:

1. Article: *We have experimented on the chemical and mechanical high-entropy alloys CoCrFeMnNi. We have also done done experiments with alloys after substituting elements,Ti for Co Mo or V for Cr. The factors affecting stability of various phases is studied.* Answer: *CoCrFeMnNi, TiCrFeMnNi, CoMoFeMnNi, CoVFeMnNi*

2. Article: *AlCrFeCoNiCuTi alloy contains BCC1 phase, BCC2 phase and a FCC phase. AlCrFeCoNiCuV alloy contains two different phases with BCC, FCC structure, respectively.*
Answer: AlCrFeCoNiCuTi, AlCrFeCoNiCuV
…

n. Article: *$Al_xTi(x=1,x=2,x=3)$ are a class of alloys used for various applications.*

Answer: AlTi, Al_2Ti, Al_3Ti

2. **Retrieval Augmented Generation:**
RAG retrieves similar examples from a pre-written collection of domain specific examples.

Article:
The high entropy arc-melted $AlCoCrCuMo_x$ (where x=0,0.3,0.5) alloy has been extensively studied to understand influence of composition of the alloy on the mechanical property. Hardness, tensile strength, fatigue resistance has been reported in this work.

Embedding of article → Similarity Search → Vector Store: Embedding of example 1 … Embedding of example n

Retrieved examples from the vector store

1. Article: *$Al_xTi(x=1,x=2,x=3)$ are a class of alloys used for various applications.*
Answer: AlTi, Al_2Ti, Al_3Ti

2. Article: *$Al_xMoCoTi_{1-x}(x=0.1,0.5,0.9)$ have been studied to understand mechanical behavior of the multi-element alloy with varied composition and temperature. The alloys exhibit a dual phase microstructure in general with FCC and BCC phases.*
Answer: $Al_{0.1}MoCoTi_{0.9}$, $Al_{0.5}MoCoTi_{0.5}$, $Al_{0.9}MoCoTi_{0.1}$

3. **Confirmation from the LLM:**

AI: Alloy composition: AlMoCuCrCo
Crystal Structure: FCC

User: Return true if the alloy AlMoCuCrCo has FCC crystal structure according to the article, else return false.

AI: false

Data extraction workflow

The decomposition of an $Al_2CoCrCuFeNi$ high-entropy alloy produced by splat quenching and casting was investigated by the analytical high resolution methods: transmission electron microscopy and three-dimensional atom probe. It could be shown that splat-quenched alloy consisted of an imperfectly ordered body-centred cubic phase with a domain-like structure, whereas normally cast alloy formed several phases of cubic crystal structure. The cast alloy decomposed into both dendrites and interdendrites. A detailed local compositional analysis carried out by atom probe within the dendrites revealed that the alloying elements in the Ni–Al-rich plates and Cr–Fe-rich interplates are not randomly distributed, but segregate and form areas with pronounced compositional fluctuations.

\+ Context + Few Shot Examples

Q1: Extract the alloy compositions mentioned in the paragraph. → LLM → $Al_2CoCrCuFeNi$

Q2: Extract the characterization technique of alloy $Al_2CoCrCuFeNi$ mentioned in the article.

Q3: Extract the processing conditions of alloy $Al_2CoCrCuFeNi$ mentioned in the article.

→ LLM → TEM, APT; Splat quenching and casting

…

The crystal structure, microstructure, density and Vickers hardness of four multi-principal element alloys, NbTiVZr, NbTiV2Zr, CrNbTiZr, and CrNbTiVZr, are reported. The alloys have been characterized using X-ray diffraction and these potential new high-temperature structural alloys are explored. The alloys were prepared by vacuum arc melting followed by hot isostatic pressing and homogenization annealing.

→ Pipeline →

Alloys	Characterization	Processing	…
$Al_2CoCrCuFeNi$	TEM, APT	SQ, AC	…
NbTiVZr	XRD	AC	…
…	…	…	…
…	…	…	…

Results and discussions

	Alloys	Characterization techniques	Processing conditions	Properties	Value	Units
1	NbMoTaW	X-Ray diffraction	Vacuum arc-melting	Yield Stress	1390	MPa
2	NbTiVZr	X-Ray diffraction	As-cast, Splat quenched	-	-	-
3	$Al_{0.5}CoCrCuFeNi$	Scanning electron microscopy, Electron dispersive spectroscopy	Arc-melting, water quenched and cold rolled	Hardness	208	HV
4	$Ti_{0.5}CrFeCoNiAl_{0.75}Cu_{0.25}$	Scanning electron microscopy	Arc-melting	Compressive strength	2697	MPa
5	$Ti_{0.5}CrFeCoNiCu$	Scanning electron microscopy	Arc-melting	Compressive strength	3135	MPa
6	$Al_{0.3}CoCr_2FeNi$	Scanning electron microscopy, X-Ray diffraction	Arc-melted and water quenched	Vickers Hardness	343	HV
7	CoCrFeMnNi	X-Ray diffraction	Arc melting	-	-	-
8	$NbTiV_2Zr$	Pyconometry, Scanning electron microscopy	Vacuum arc melting, hot isostatic pressing	Density	6340	kg/m^3
9	$Al_{0.7}CoCrFeNi$	Scanning electron microscopy	Vacuum arc melting, hot isostatic pressing	Ultimate tensile strength	1400	MPa
…	…	…	…	…	…	…
n	$Al_{0.2}Co_{1.5}CrFeNi_{1.5}Ti$	SEM, EDS, XRD	Arc-melting, aging	Wear resistance	5500	m/mm^3

Data extracted from academic works of multi-element alloys

- To evaluate our model, we compute:

$$\text{Recall}=\frac{|\{\text{relevant entries}\}\cap\{\text{retrieved entries}\}|}{|\{\text{relevant entries}\}|} \qquad \text{Precision}=\frac{|\{\text{relevant entries}\}\cap\{\text{retrieved entries}\}|}{|\{\text{retrieved entries}\}|}$$

$$\text{F1-Score}=\text{Harmonic\_mean}(\text{Precision}, \text{Recall})$$

- We tested our framework on papers on multi-element alloys

MODELS:	GPT-3.5 turbo	GPT-3.5 turbo with confirmation	GPT-3.5 turbo with RAG and confirmation	GPT-4o with RAG and confirmation	GPT-4o with RAG and without confirmation	GPT-4o mini with RAG and without confirmation
Alloys	0.70	0.90	0.87	0.92	0.96	0.92
Processing Conditions	0.80	0.87	0.84	0.91	0.96	0.81
Characterization techniques	0.63	0.88	0.83	0.82	0.99	0.93
Properties	0.86	0.83	0.89	0.75	0.89	0.94

F1 Scores for our experiments with various LLMs on works from multi-element alloys

	Alloys	Processing Conditions	Characterization techniques	Properties
Precision	1	1	1	0.88
Recall	0.93	0.92	0.98	0.90
F1-Score	0.96	0.96	0.99	0.89

GPT-4o mini with RAG

	Alloys	Processing Conditions	Characterization techniques	Properties
Precision	1	0.77	0.93	0.95
Recall	0.86	0.85	0.93	0.93
F1-Score	0.92	0.81	0.93	0.94

GPT-4o with RAG

Analysis of the best models for the multi-element alloy data extraction task

MODELS:	GPT-3.5 turbo	GPT4o-mini	GPT4o
Cost per paper	$0.03	$0.003	$0.15

- Data extraction using Openai's LLMs take around 30 seconds per article.
- Automated data extraction takes significantly lesser time and performs reliably.

Future work

- Extraction of materials' data from a collection of 18000 academic works on multi-element alloys.
- Data extraction from figures and other forms of data present in the papers.
- Exploration of RAG for context retrieval, and exploration of fine-tuning to improve performance.

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