

A Brief Overview of Citrine's Data and Informatics Platform

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Citrine Informatics

CHiMaD Meeting
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The Citrine Platform Architecture



Shinier Paint



Tougher Phones



Lighter Vehicles



Greener Suppliers

Machine Learning and Apps

Citrine and third parties can build powerful analytics for physical product companies

World's Largest Physical Data Platform

Citrine is consolidating vast stores of physical knowledge

Data Extraction from Documents

Citrine's extraction engine ingests quantitative data from research papers, patents, data sheets

Data Streaming from Users

Customers and a growing network of government and university labs push data to our platform

The Industrial Materials Design Problem

CUSTOMER PROJECT: FORMULATION DEVELOPMENT

90

possible
physical inputs

35

product features
need optimization

10^{89}

combinations represent
overwhelming search
space

Global Leaders Choose Citrine

Aerospace



Materials

Fortune 200
materials co.

Defense



Electronics

Panasonic

Automotive



Alloys



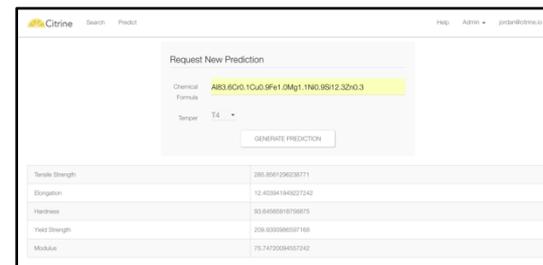
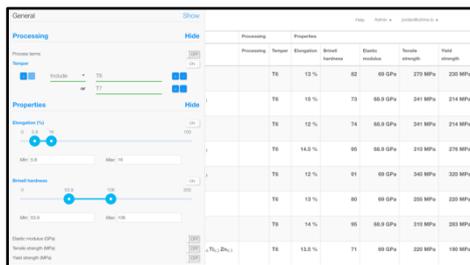
Large-Scale Data and AI for All Materials

Thermoelectrics



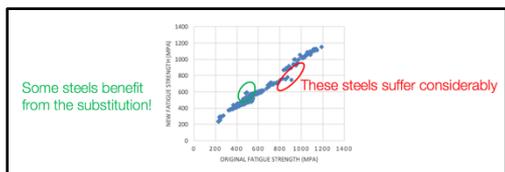
25k precomputed & 1.5k user-requested materials
Users at NASA, LBNL, MIT

Aluminum Alloys



World's largest ML-ready Al alloy database
AI-based models of properties

Steel



Web-based models for real-time steel design

Plus customer use cases: coatings, energy materials, epitaxy, next-generation aerospace alloys, ...

Missing Link in the Materials Genome

Real-time, easy-to-use, web-based data infrastructure and predictive tools

A metallurgist can go to
citrination.com/alloys/predict
and input composition and temper

In a few seconds, user receives AI output
No programming, learning curve, or waiting

Request New Prediction

Chemical Formula

Temper

Request New Prediction

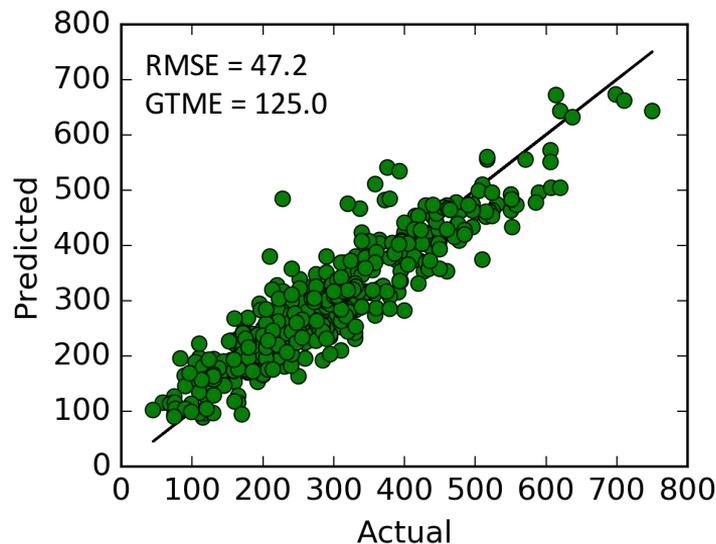
Chemical Formula

Temper

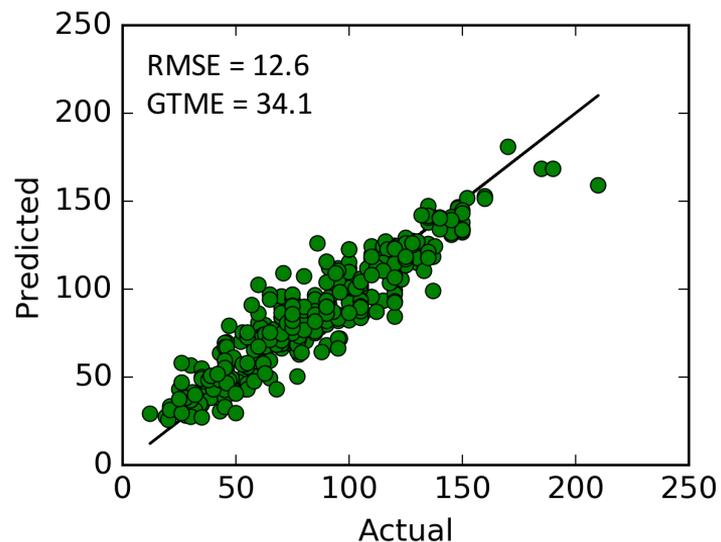
Tensile Strength	422.13955479644636
Elongation	13.072276636619629
Hardness	115.24441342594316
Yield Strength	316.5495388684673
Modulus	76.0

AI-Based Models Are Very Accurate

Tensile Strength



Hardness



One organization that has made significant progress in establishing a centralized data resource for materials scientists is **Citrine Informatics**, a company that specializes in applying data mining to materials discovery and optimization.

— *Ceder, Jain, Persson*

APL Materials

<http://dx.doi.org/10.1063/1.4944683>

Statistics on Citrination.com

Search Data

Welcome to Citrination. The Search Data page allows you to find tabulated materials property data. These are data that users have contributed or Citrine has automatically extracted from literature. [Make a contribution.](#)

binary oxide bulk modulus

10 1 to 10 of 3014260 total

Prev Next

Material	Property	Value	Conditions	Reference
BeO	Bulk modulus VRH average, K_{VRH}	208.348306646 GPa	Data type: Computational Materials Project ID: mp-2542 Space group: 186 Unit cell volume: 27.975749228 Å ³ +1 more...	<ul style="list-style-type: none">M. de Jong, et al., Scientific Data 2, 150009 (2015) Contributed by: bryce@citrine.io
BeO	Isothermal bulk modulus	219 GPa	Phase: Hexagonal	<ul style="list-style-type: none">V. Milman and M. C. Warren, Journal of Physics: Condensed Matter 13, 241 (2001) Contributed by: Citrine
BeO	Bulk modulus K_0	224.4 GPa	Crystal system: hexagonal Crystallinity: single crystal Structure: Wurtzite Temperature: room temperature +2 more...	<ul style="list-style-type: none">C. F. Cline, Journal of Applied Physics 38, 1944 (1967) Contributed by: David M. Teter

3.1m free data records

Users from almost 2k institutions worldwide



Data Extraction: Text

Kinetics of premartensite to martensite transition and its implications on the origin of modulation in Ni₂MnGa ferromagnetic shape memory alloy

Sanjay Singh¹, J. Bednarek², S. R. Barman¹, C. Felser¹, and Dhananjai Pandey⁴

¹Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Strasse 40, D-01187 Dresden, Germany

²Photon Sciences, FS-PE, Deutsches Elektronen Synchrotron (DESY), 22607 Hamburg, Germany

³UGC-DAE Consortium for Scientific Research, Khandwa Road, Indore, 452001, India.

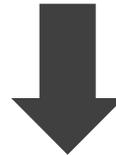
⁴School of Materials Science and Technology, Indian Institute of Technology (Banarus Hindu University), Varanasi-221005, India.

Abstract

We present here results of temperature dependent high resolution synchrotron x-ray powder diffraction study of sequence of phase transitions in Ni₂MnGa. Our results show that the incommensurate martensite phase results from the incommensurate premartensite phase, and not from the austenite phase assumed in the adaptive phase model. The premartensite transforms to the martensite phase through a first order phase transition with coexistence of the two phases in a broad temperature interval (~40K), discontinuous change in the unit cell volume as also in the modulation wave vector across the transition temperature and considerable thermal hysteresis in the characteristic transition temperatures. The temperature variation of the modulation wave vector q shows smooth analytic behavior with no evidence for any devilish plateau corresponding



confirms the cubic structure in the Fm-3m space group (see Fig 3a). The cell parameter ($a=5.82445(1)$ Å) obtained by us is in good agreement with those reported by earlier workers. [7, 11]



cell parameter a = MATERIALS PROPERTY
5.82445(1) = NUMERICAL VALUE
angstrom = UNITS



Extraction: Images & Tables

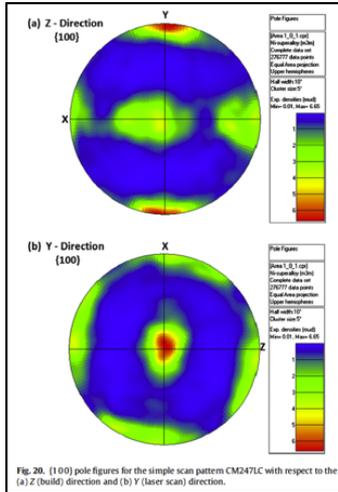


Image: **0.84**
 Plot: **0.06**
 Table: **0.10**

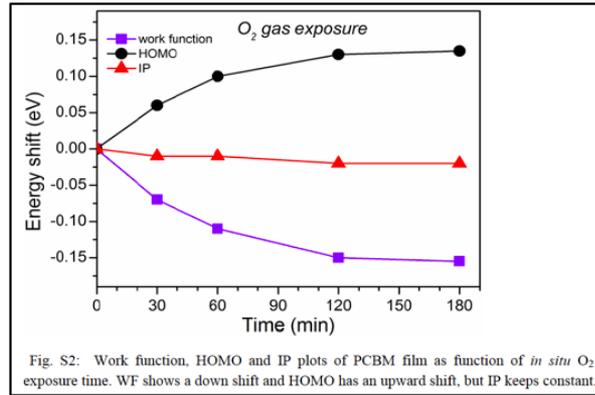


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 Plot: **0.94**
 Table: **0.04**

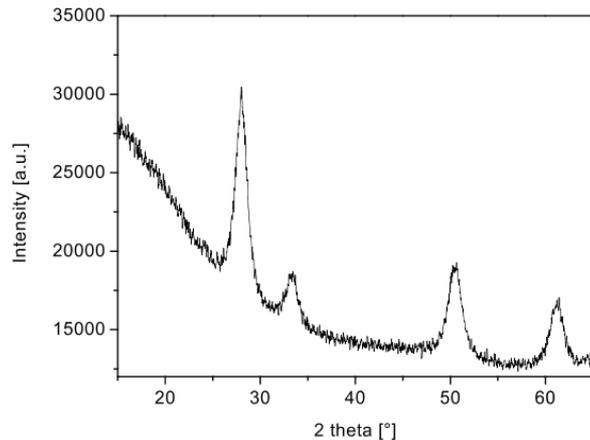
p_c	Method	Reference
Nishimori point in the $\pm J$ model		
0.111 ± 0.002	Transfer matrix	[30]
0.114 ± 0.003	Series expansion	[17]
0.1128 ± 0.0008	Non-equilibrium	[31]
0.1095 ± 0.0005	Transfer matrix	[18]
0.1094 ± 0.0002	Transfer matrix	[15]
0.1093 ± 0.0002	Fermionic transfer matrix	[19]
0.110028	Duality	[21]
≤ 0.178203	Rigorous upper bound	[32]
$T = 0$ critical point in the $\pm J$ model		
~ 0.099	Series expansion	[22]
0.105 ± 0.01	Matching algorithm	[23]
$0.095 < p_c < 0.108$	Matching algorithm	[24]
0.104 ± 0.001	Exact ground states	[25]
0.106 ± 0.002	Exact ground states	[27]
0.115	Ground state enumeration	[27]
0.1031 ± 0.0001	Exact ground states	[12]
0.103 ± 0.001	Exact ground states	[28]

Image: **0.02**
 Plot: **0.00**
 Table: **0.98**



Extraction: Images & Tables

Image containing data

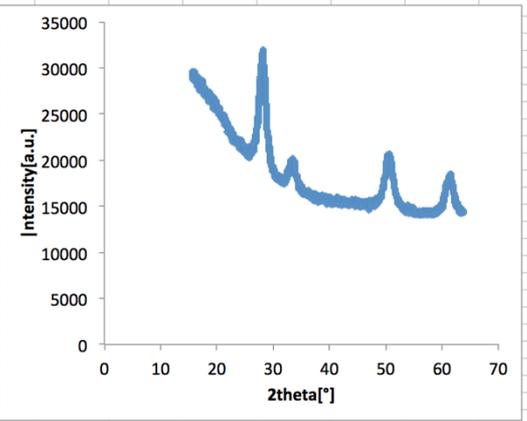


machine vision



2theta[°]	Intensity[a.u.]
28.113381	32034.0536
28.113381	31965.0781
28.113381	31896.1026
28.113381	31827.1271
28.113381	31758.1516
28.113381	31689.1762
28.113381	31620.2007
28.0006952	31551.2252
28.113381	31551.2252
28.0006952	31482.2497
28.113381	31482.2497
28.0006952	31413.2742
28.113381	31413.2742
28.0006952	31344.2987
28.113381	31344.2987
28.0006952	31275.3232
28.113381	31275.3232
28.0006952	31206.3477
28.0006952	31137.3722
28.2260668	31137.3722
28.0006952	31068.3967
28.2260668	31068.3967
28.0006952	30999.4212
28.2260668	30999.4212
28.0006952	30930.4457
28.2260668	30930.4457

Underlying x,y data
(*actual extraction shown*)



Extraction in Production Today

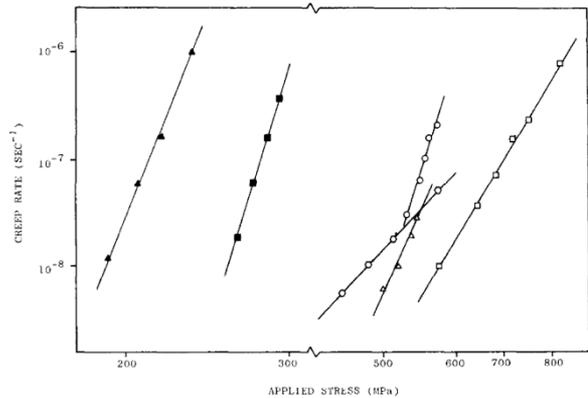


Fig. 1. The creep rates as a function of applied stress at 760 °C: ▲, MA 754; ■, MA 753; ○, MA 6000E; △, Nimonic 115; □, Mar M200; ◊, Udimet 700.

Material	Property	Value	Conditions	Reference	Actions
MA 754	Creep rate	$1.1\text{e-}07$ to $9.7\text{e-}06$ s ⁻¹	Applied stress: 191.45 to 235.71 MPa Temperature: 760 °C	<ul style="list-style-type: none"> The Role of the Alloy Matrix in the Creep Behaviour of Particle-strengthened Alloys; Materials Sciences and Engineering 44 (1980) 165-172 Contributed by: Jo	
MA 753	Creep rate	$1.8\text{e-}07$ to $3.5\text{e-}06$ s ⁻¹	Applied stress: 264.07 to 292.75 MPa Temperature: 760 °C	<ul style="list-style-type: none"> The Role of the Alloy Matrix in the Creep Behaviour of Particle-strengthened Alloys; Materials Sciences and Engineering 44 (1980) 165-172 Contributed by: Jo	



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Abstract
Keywords
1. Introduction
2. Software and structure database
3. Basic operation
4. Structure analysis tools
5. Example applications
6. Future developments: high-throughp...
7. Summary
Acknowledgments
References

Figures and tables

Computational Materials Science
Volume 58, June 2012, Pages 218–226

AFLOW: An automatic framework for high-throughput materials discovery

Stefano Curtarolo^{a, b, *}, Wahyu Selyawan^a, Gus L.W. Hart^c, Michal Jahnatek^a, Roman V. Chepulskii^a, Richard H. Taylor^a, Shidong Wang^a, Junkai Xue^a, Kesong Yang^a, Ohad Levy^d, Michael J. Mehl^a, Harold T. Stokes^e, Denis O. Demchenko^f, Dane Morgan^a

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Cite this: DOI: 10.1039/c5ee03488d

Development of solar fuels photoanodes through combinatorial integration of Ni–La–Co–Ce oxide catalysts on BiVO₄†

D. Guevarra,^{‡a} A. Shinde,^{‡a} S. K. Suram,^a I. D. Sharp,^{bc} F. M. Toma,^{*bc} J. A. Haber^{*a} and J. M. Gregoire^{*a}

Acknowledgements

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