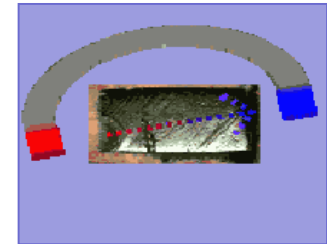


凝聚态物理-北京大学论坛

新型磁相变材料设计 和物性调控

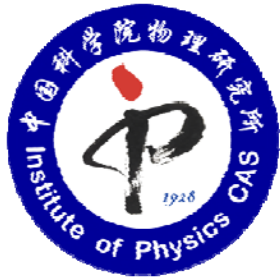


王文洪

磁学国家重点实验室 M05组
中国科学院物理研究所

2016. 10. 27





磁学国家重点实验室

磁电子学物理和材料

纳米结构材料和物理

稀土合金和氧化物磁性材料和物理

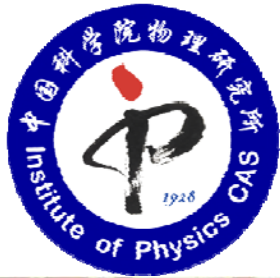
新型磁性功能材料探索和物理

多铁材料和物理

磁记录材料和物理



IOP, CAS



新型磁性功能材料



研究员 2

副研究员 2

高级实验师 1

工程师 1

学生 10



研究内容

- 1) **Heusler** 型立方结构磁相变材料
- 2) **MMX** 六角结构合金磁相变材料
- 3) 量子电子学材料
- 4) 拓扑绝缘体金属间化合物
- 5) 基于波谱学的物性研究



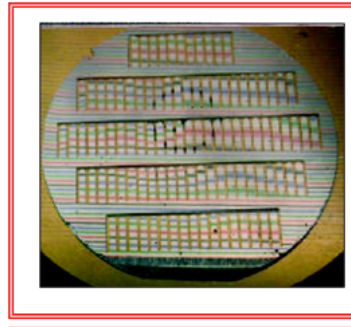
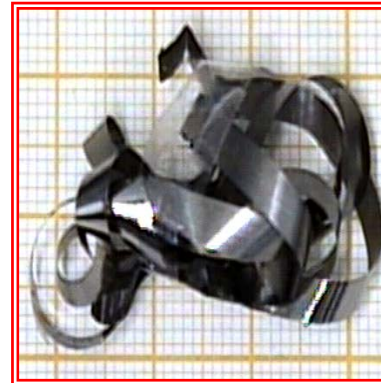
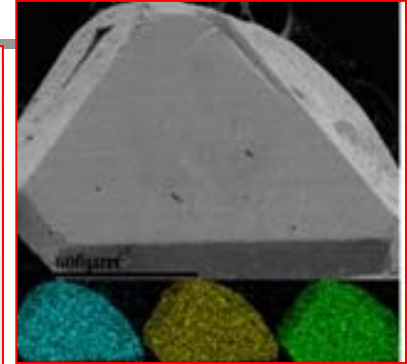
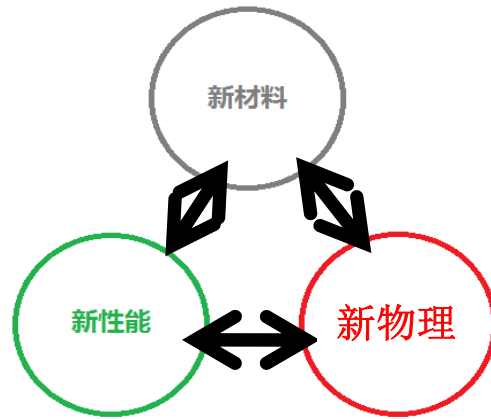
研究思路和技术特色

以新材料为基点，知识产权，新现象，新性质，新物理

相信传统物质里面有新材料

一个成分多种物相

做块体材料容易调整成分



报告内容

■ 研究背景

1. 马氏体相变-形状记忆效应
2. 磁性马氏体相变-铁磁形状记忆效应
3. 磁驱动马氏体相变-磁驱动效应

■ 新型磁相变材料设计和物性调控

1. $\text{Mn}_{1-x}\text{CoGe}$ -空位调控居里温度窗口
2. MnNiGe:Fe -等结构合金化构建温度窗口
3. MnNiGa -磁性和化学键调控磁性斯格明子

■ 致谢

传统形状记忆合金：NiTi

眼镜架



人工关节



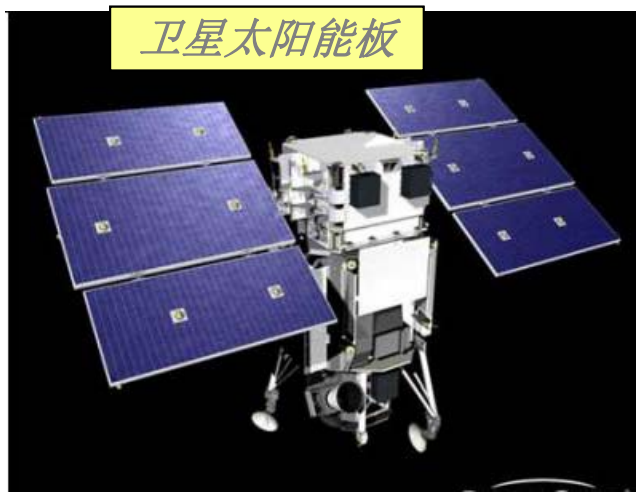
管道接口



航天飞机天线



卫星太阳能板



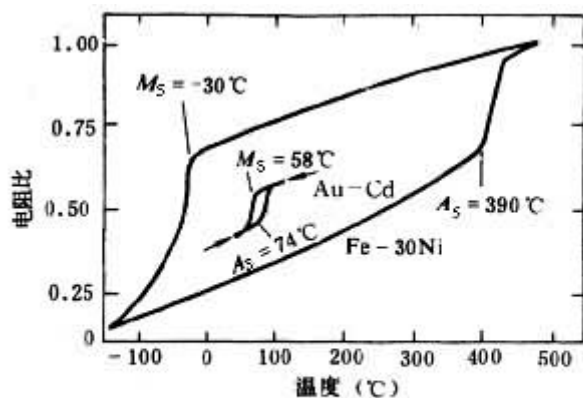
合金具有“记忆”的原因？

形状记忆依赖于马氏体相变

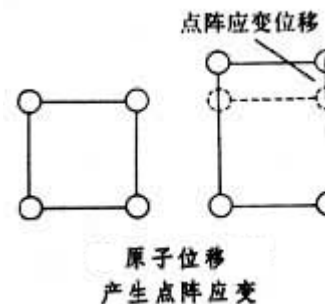
马氏体相变：非原子扩散型结构对称性的改变，一级相变

Bain模型：立方→四方

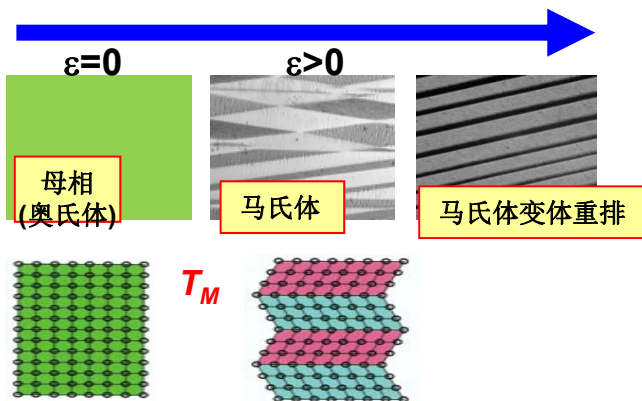
温度或应力诱发：伴随发生应变和电阻等物理量的变化



Fe-Ni 和 Au-Cd 合金的相变热滞
 M_s : 马氏体转变开始温度 A_s : 马氏体逆变开始温度



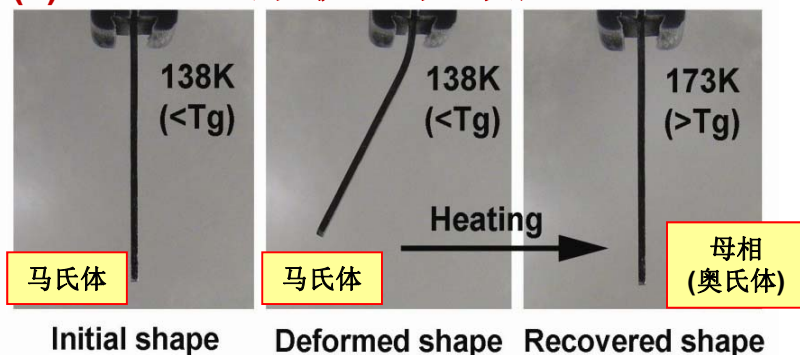
降低温度或增加外应力



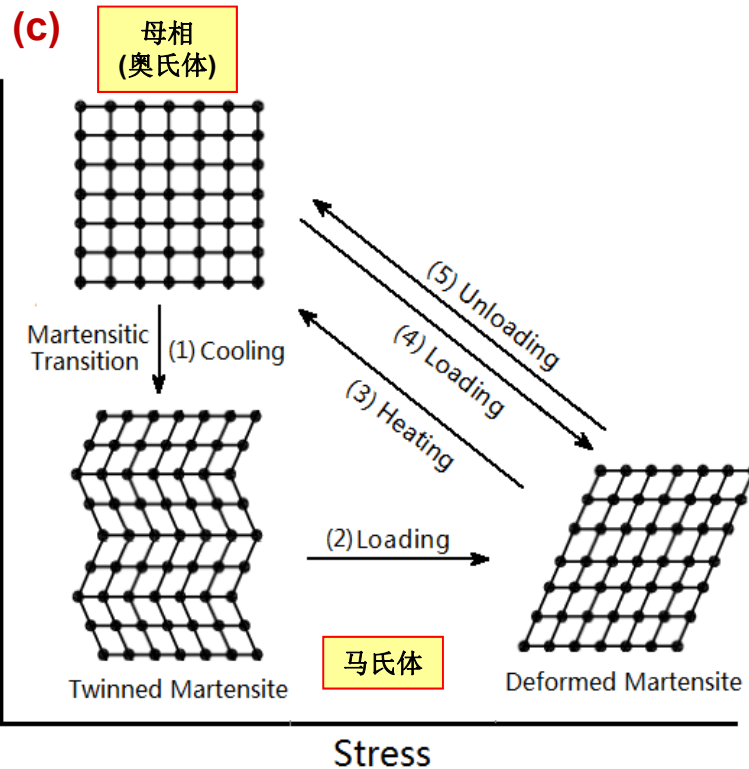
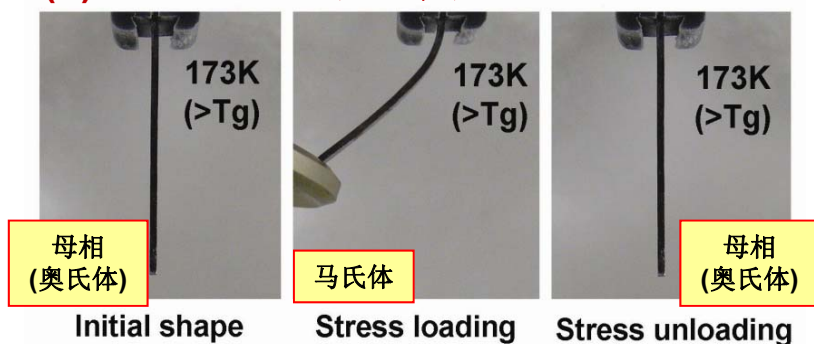
升高温度或去掉外应力

形状记忆效应和超弹性

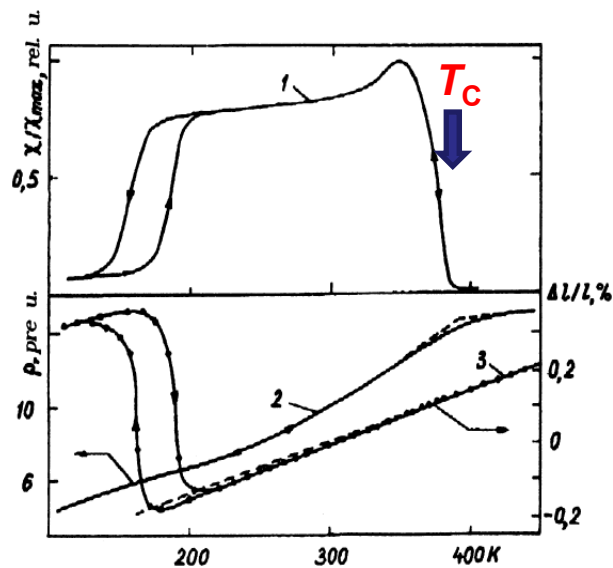
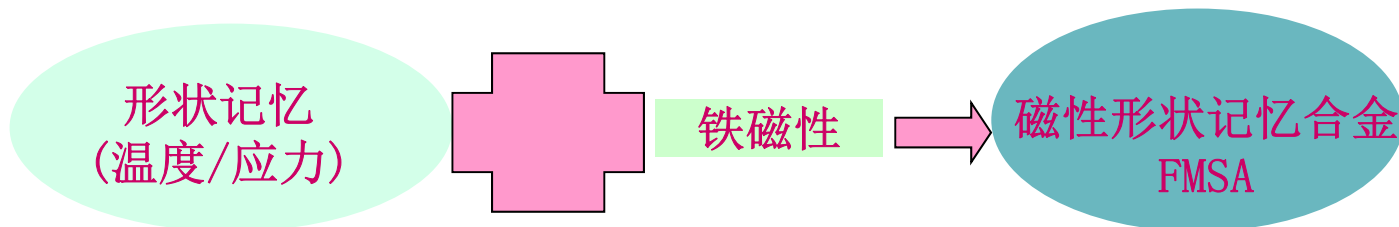
(a) 形状记忆效应



(b) 超弹性



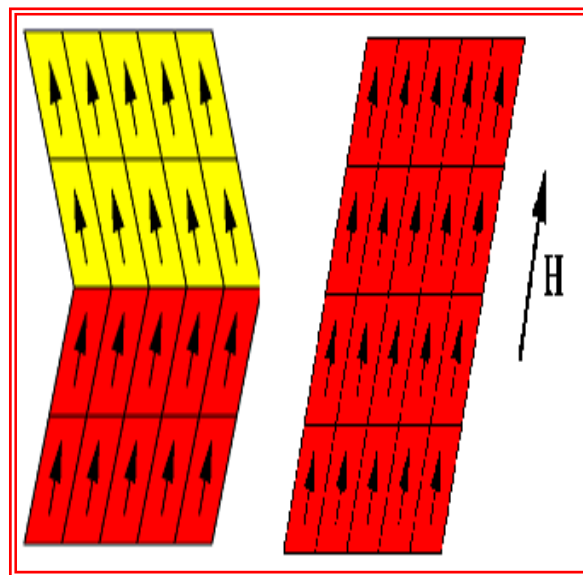
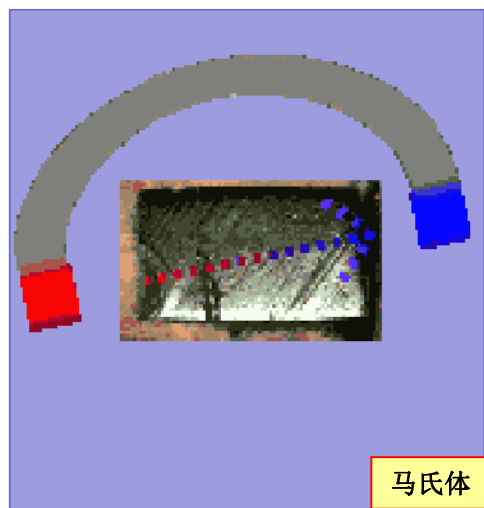
铁磁形状记忆合金



Chernenko, et al. Phys. Met. Metall. 1989.

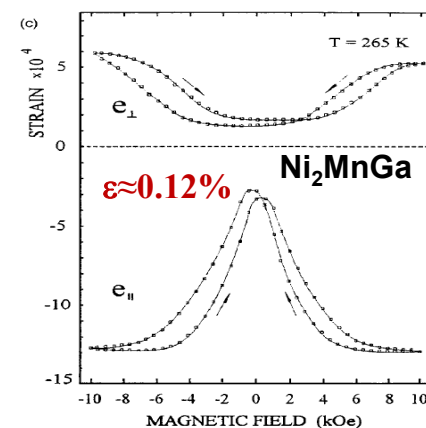
晶体结构转变和磁结构转变耦合发生

磁驱大应变

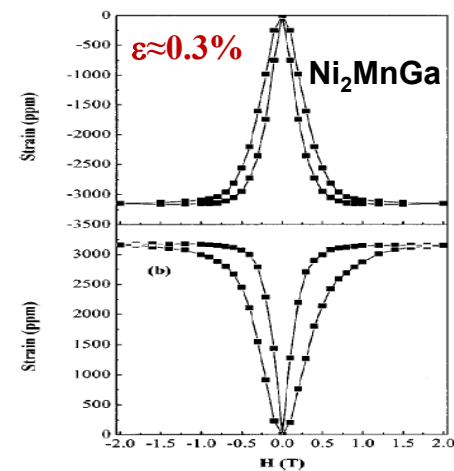


磁场来影响马氏体变体取向

O'Handley et al. APL, 1996



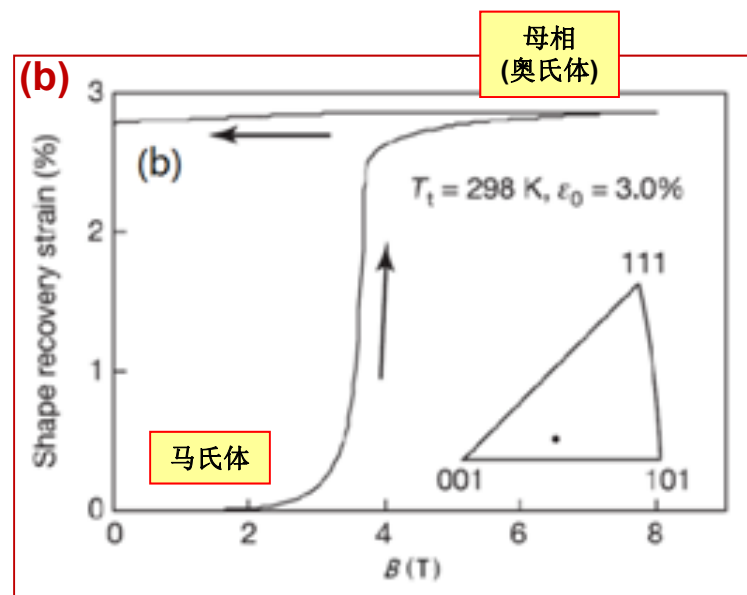
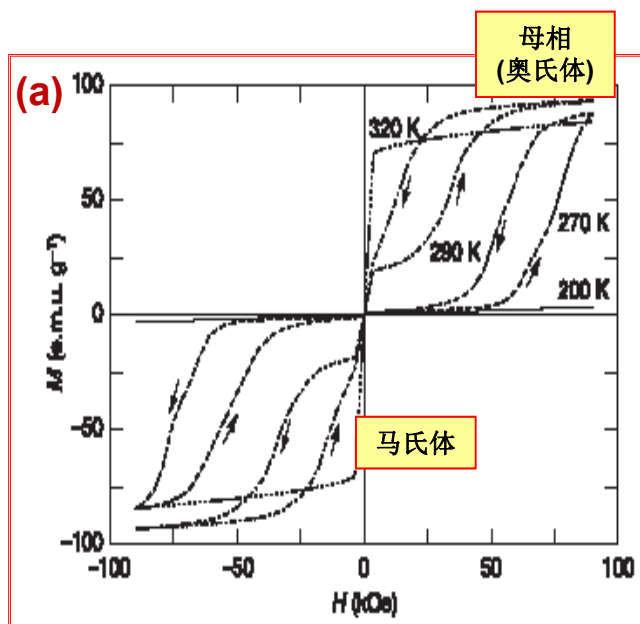
G.H.Wu, et al. APL, 1999



磁驱动马氏体相变 (Heusler alloys)

◆ NiMnIn:Co

◆ 2006年日本 Kainuma

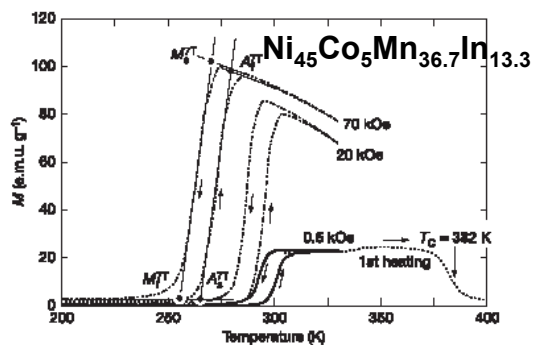


Jpn: Nature 2006

磁驱动效应 (Heusler alloys)

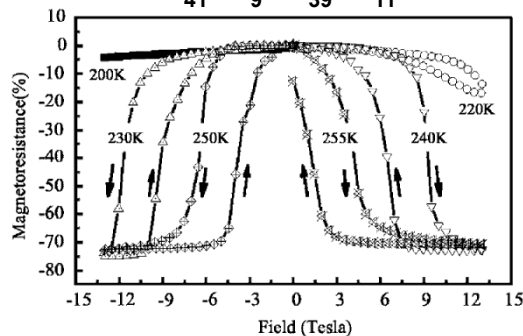
磁驱动形状记忆

R. Kainuma, et al. Nature, 2006.



磁电阻

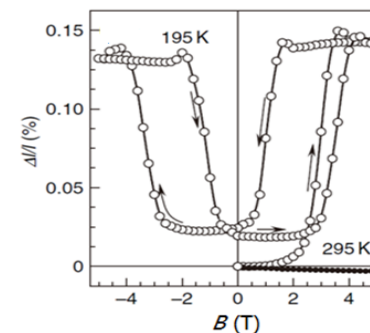
S.Y.Yu, G.H.Wu, et al. APL, 2007



磁驱超弹性

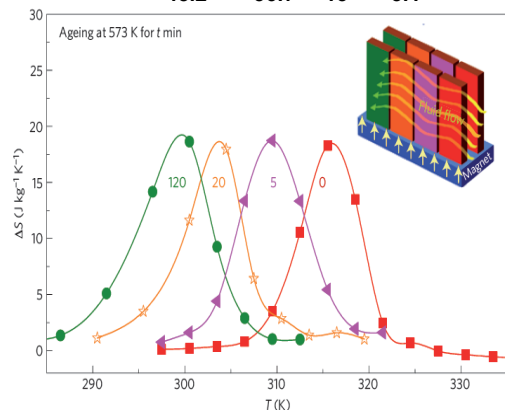
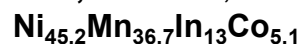


T. Krenke, et al. PRB, 2006



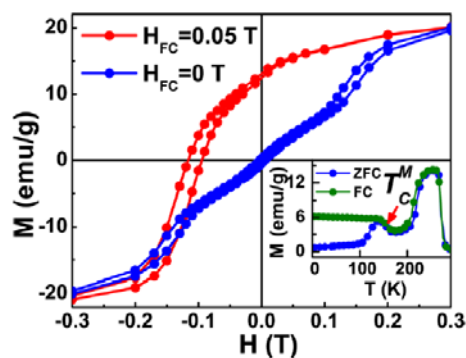
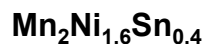
磁熵变

J.Liu, et al. NM, 2013



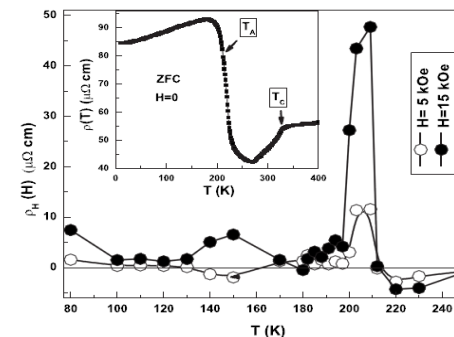
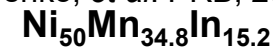
交换偏置

L.Ma, G.H.Wu, et al. APL, 2011

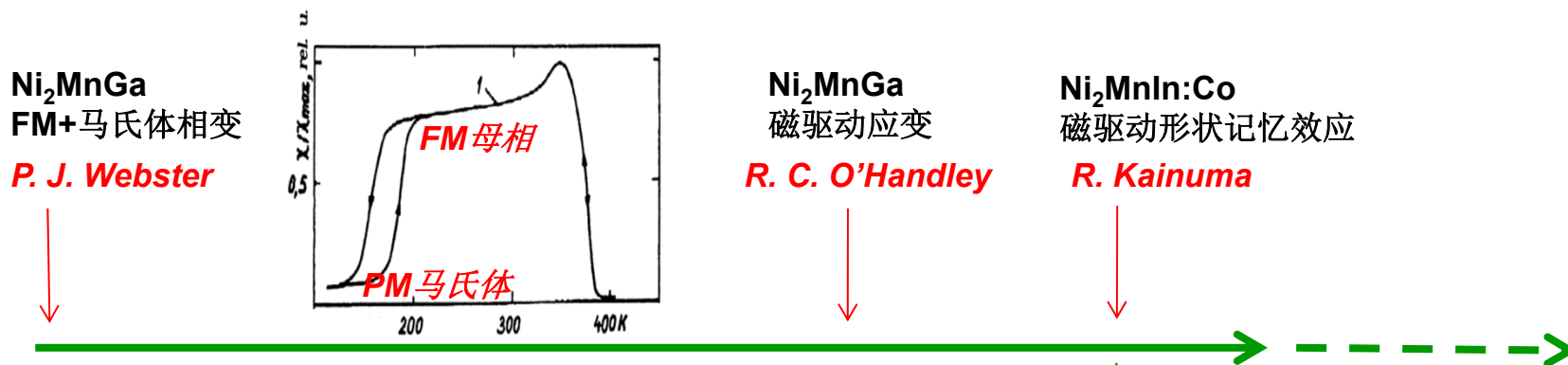


霍尔效应

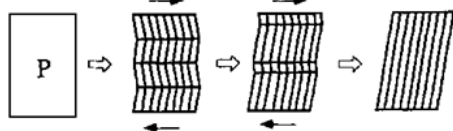
I. Dubenko, et al. PRB, 2009



磁相变材料研究历程 (Heusler alloys)



1968

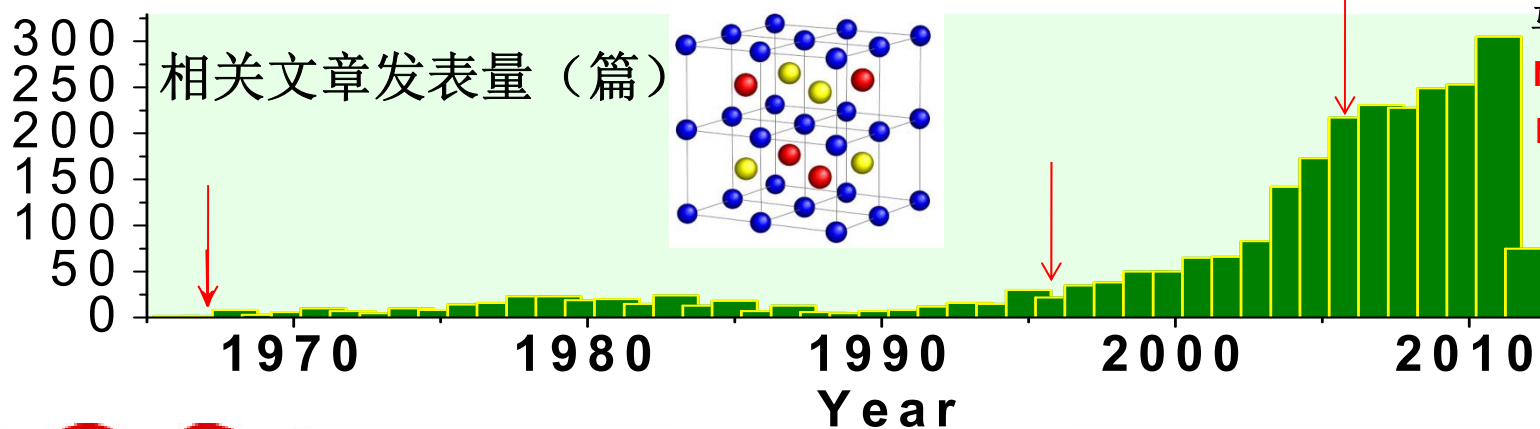


1996

Ni_2MnGa
磁驱动大应变
吴光恒

2006

$Ni_2MnSb:Co$
 $Ni_2MnGa:Co$
磁驱动形状记忆效应
吴光恒



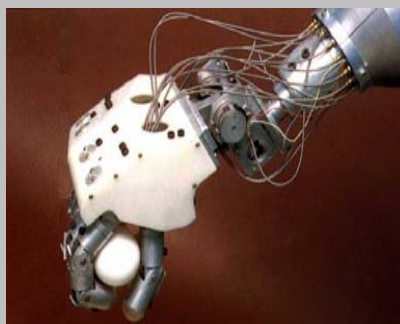
马氏体相变体系:
 Ni_2FeGa (柳祝红)
 Mn_2NiGa (刘国栋)
 Fe_2MnGa (朱伟)

磁相变材料的应用

智能器件



微型线性马达



磁驱动机器手

绿色能源



2016夏季奥运会开启制冷界的一场革命 - 环境友好的磁冰箱问世

磁制冷冰箱

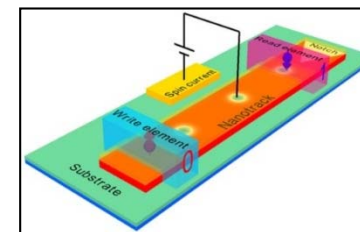


热磁发电装置

自旋电子学器件



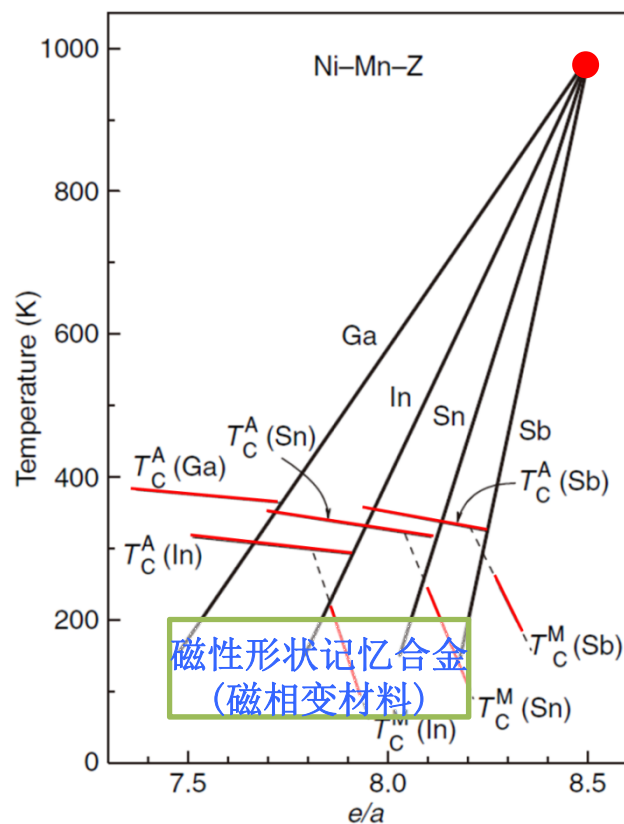
磁信息存储



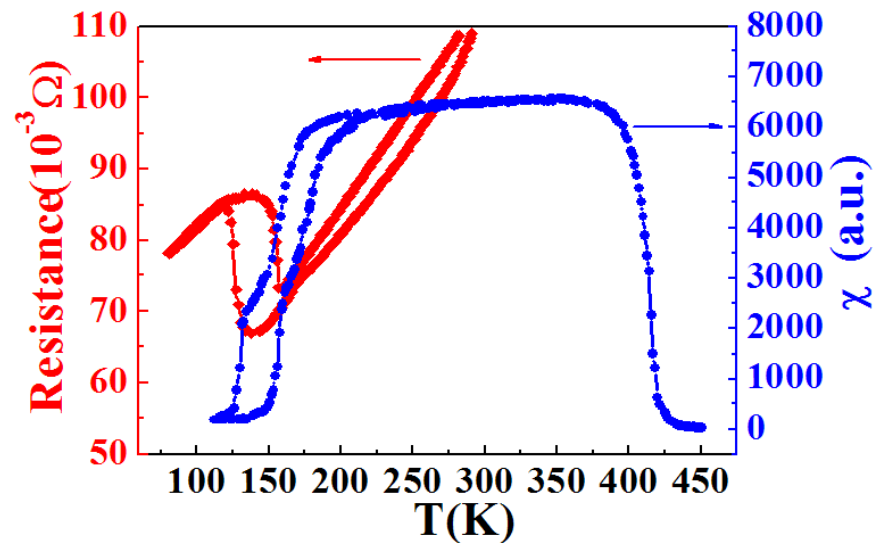
电流驱动 (电控磁)

磁驱相变的条件 (Heusler alloys)

晶体结构转变和磁结构转变耦合发生 (第一条件)



Aksoy, S., et al. *Phil. Mag.* 2009, 89: 2093.



磁场主动影响马氏体相变及相关物性

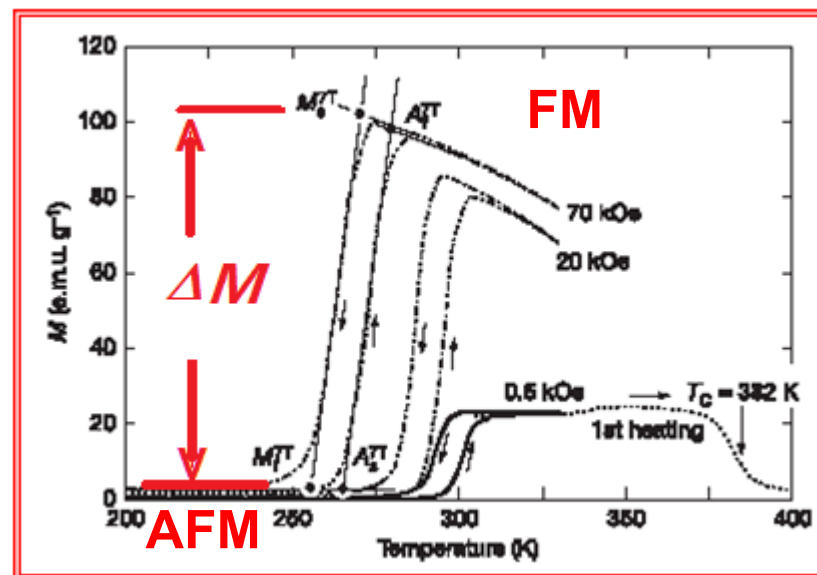
磁驱相变的条件 (Heusler alloys)

大 ΔM 是获得磁驱动效应的一个重要前提 (第二条件)

$$\frac{\Delta T}{\Delta H} = -\frac{\Delta M}{\Delta S}$$

磁场促进高磁性相的形成

R. Kainuma, *et al.* Nature, 2006.

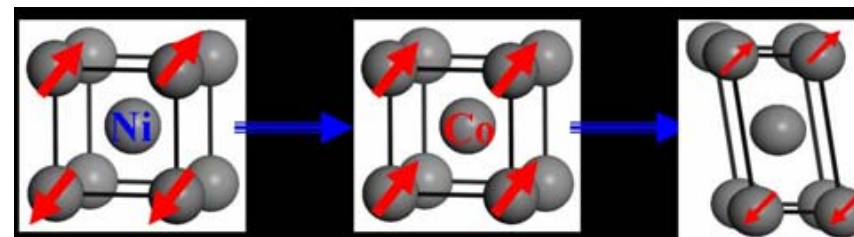
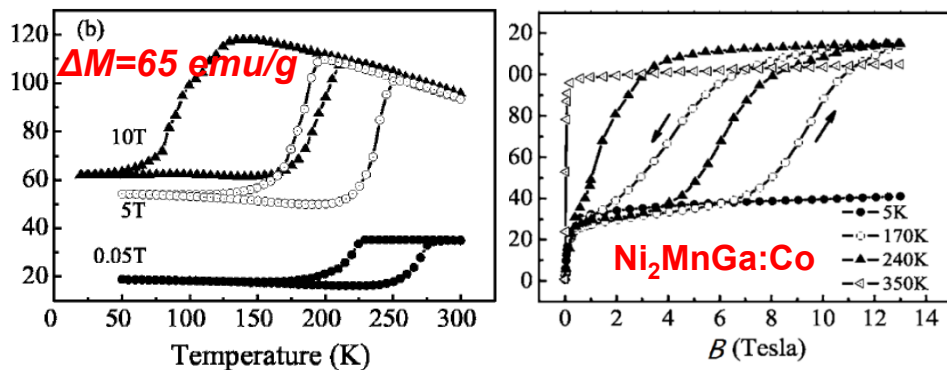


$\Delta M = 100$ emu/g

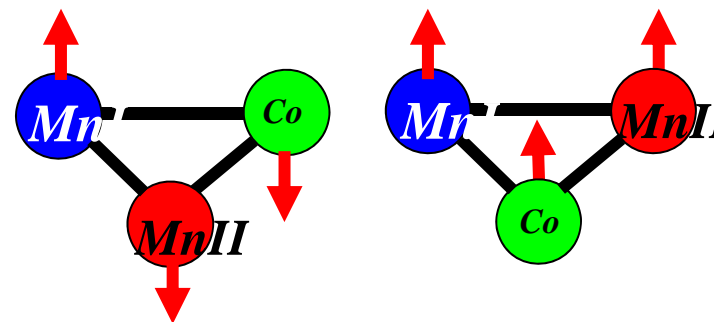
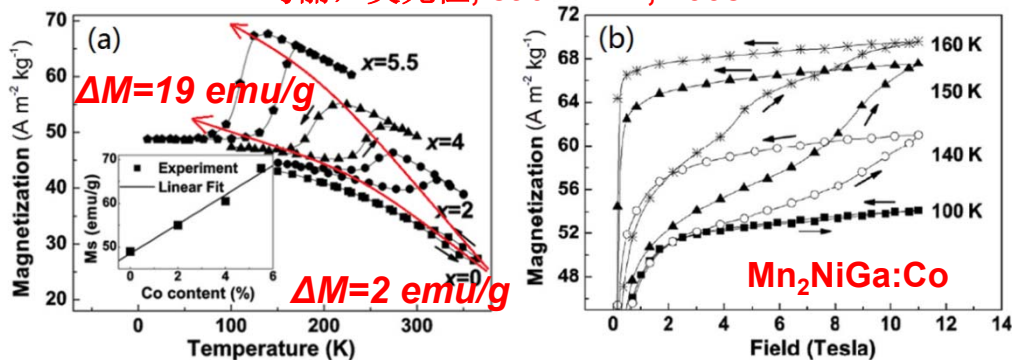
$\text{Ni}_{45}\text{Co}_5\text{Mn}_{36.7}\text{In}_{13.3}$

Co的铁磁激活效应 (Heusler alloys)

于淑云, 吴光恒, et al. APL, 2007



马丽, 吴光恒, et al. APL, 2008

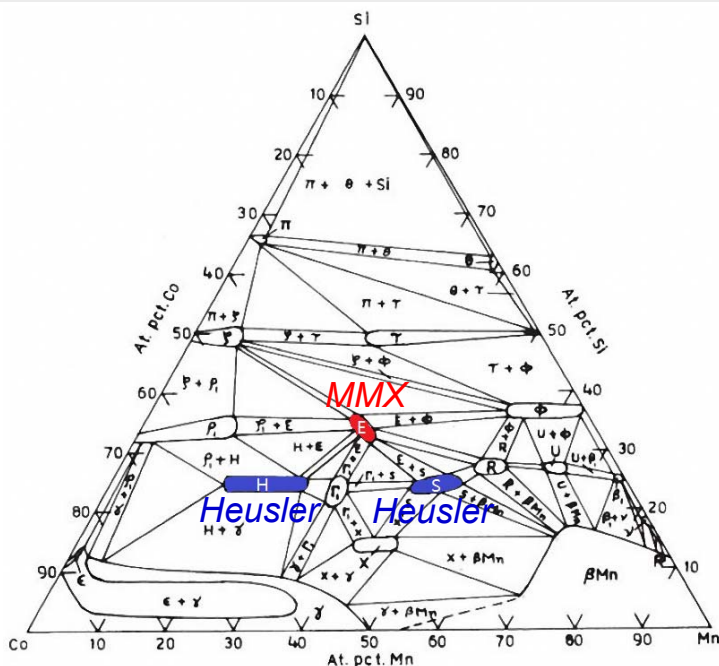


Co翻转Mn-Mn反铁磁
获得大 ΔM

为什么做MM'X合金？

- ◆ 磁场驱动相变的各种应用需要更多新材料
- ◆ Heusler型合金磁熵变和相变熵变符号相反，吸放热效应相互抵消

MM'X合金

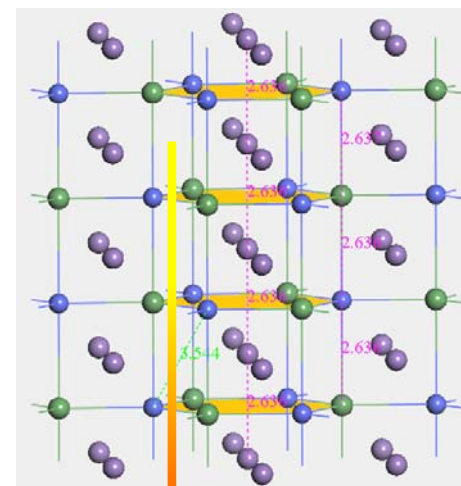


Candidate elements for MM'X compounds

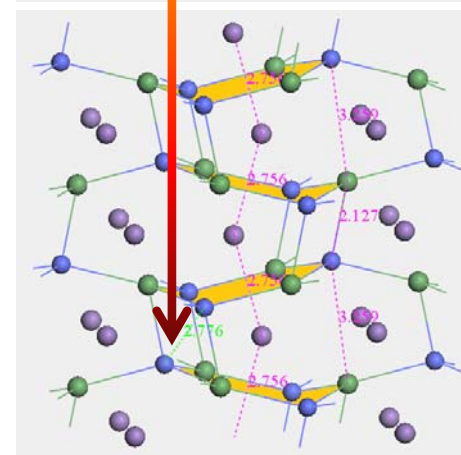
III B	IV B	V B	VI B	VII B	VIII B	IX B	X B	I B	II B	III A 13	IV A 14	V A 15
3	4	5	6	7	8	9	10	11	12	13 Al 铝	14 Si 硅	15 P 磷
21 Sc 钪	22 Ti 钛	23 V 钒	24 Cr 铬	25 Mn 锰	26 Fe 铁	27 Co 钴	28 Ni 镍	29 Cu 铜	30 Zn 锌	31 Ga 镓	32 Ge 锗	33 As 砷
39 Y 钇	40 Zr 锆	41 Nb 铌	42 Mo 钼	43 Tc 锝	44 Ru 钌	45 Rh 铑	46 Pd 钯	47 Ag 银	48 Cd 镉	49 In 铟	50 Sn 锡	51 Sb 锑
57-71 镧系	72 Hf 铪	73 Ta 钽	74 W 钨	75 Re 铼	76 Os 锇	77 Ir 铱	78 Pt 铂	79 Au 金	80 Hg 汞	81 Tl 铊	82 Pb 铅	83 Bi 铋

MnCoGe,
MnNiGe,
MnCoSi,
MnNiSi,
MnCoSn,
FeNiGe,
FeCoGe,
MnFeGe,
CrCoGe,
ZrMnGe,
...

Ni₂In-type 六角结构



母相
(奥氏体)



马氏体

TiNiSi-type 正交结构

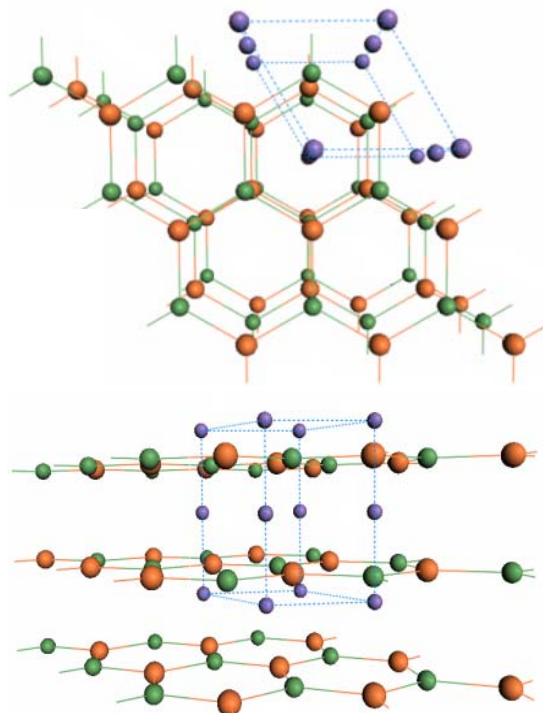
结构、占位和磁性

有序占位原则，
共价键，
磁矩

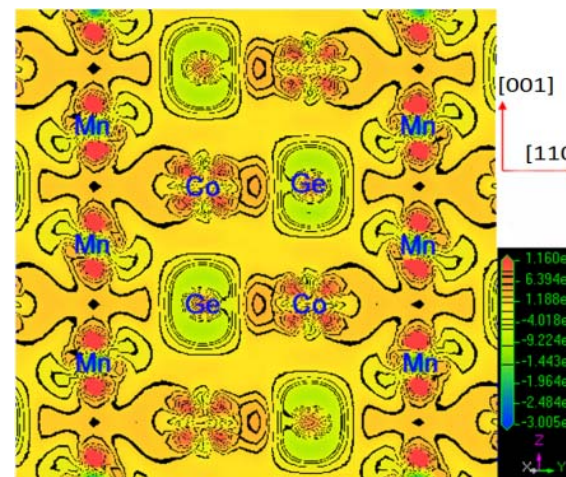
25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge
锰	铁	钴	镍	铜	锌	镓	锗
●	●	●	●	●	●	●	●



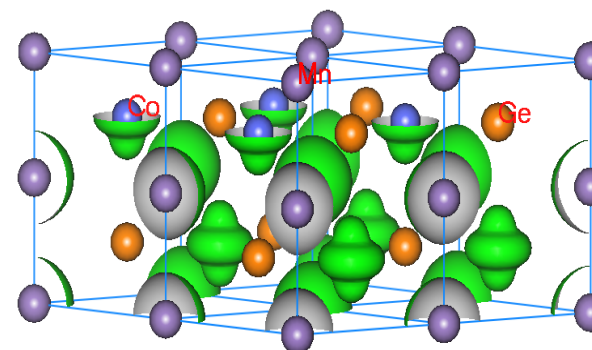
○ ○ ○



差分电子密度
(第一原理计算)

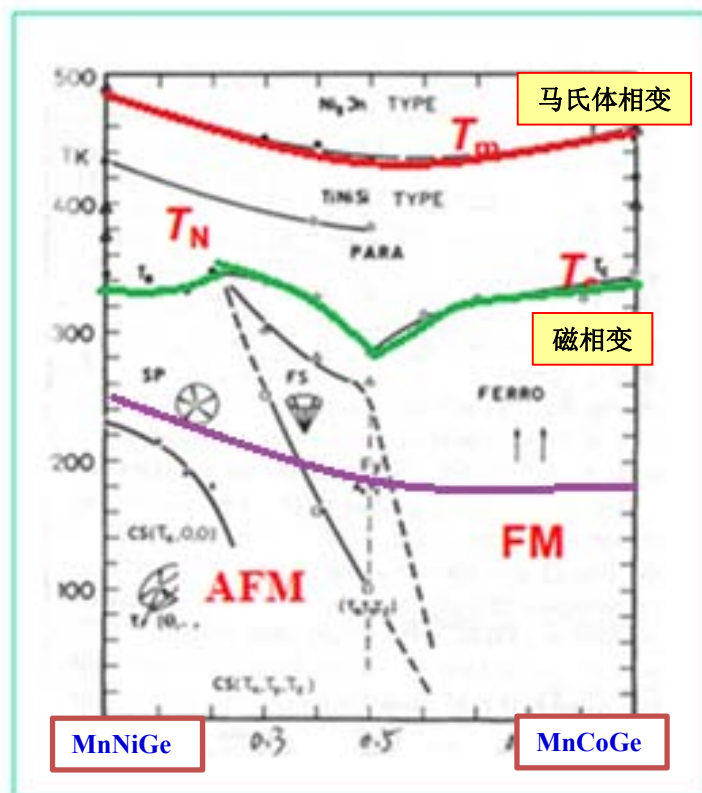


MnCoGe六角母相(110)晶面差分电子密度图



MnCoGe高温六角结构中的磁矩分布

MnNiGe & MnCoGe



Niziol, S., et al. JMMM, 1982.

◆ T_C 和 T_N 相对稳定，低温相磁性已知

◆ 反铁磁，螺旋反铁磁，锥形铁磁，铁磁

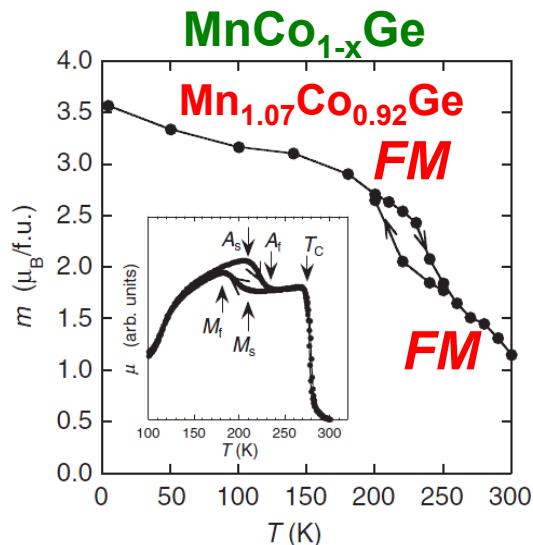
◆ Mn 为主要磁性来源

◆ 高温相磁性不清楚

◆ 高温相 T_C 低，低温相 T_C 高

$T_m > T_N$ & T_C
不是磁相变材料

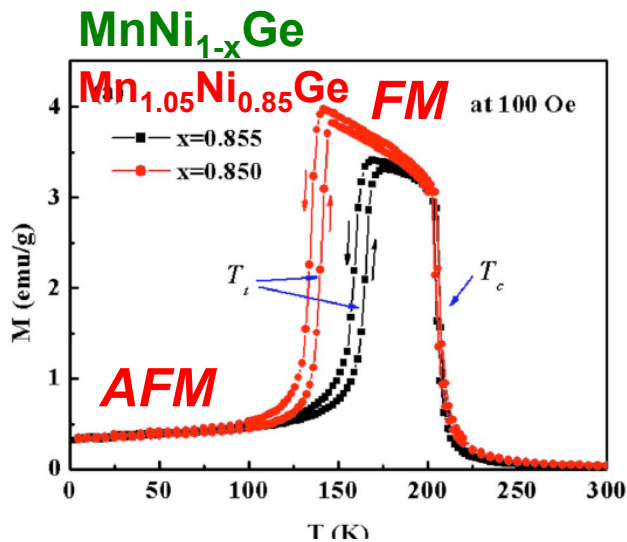
MM'X合金



Koyama K, et al. JJAP, 2004

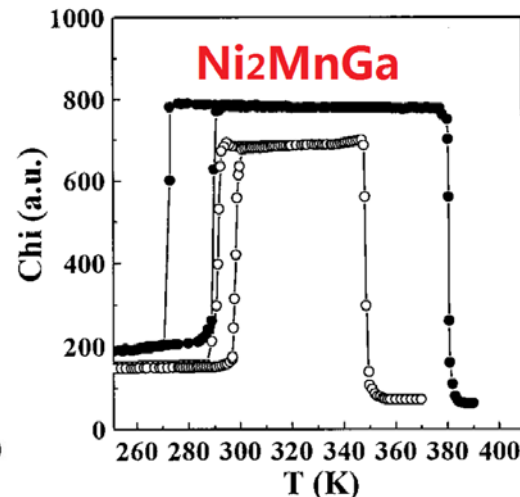
首次提出铁磁形状记忆合金

从磁驱相变的角度，
MM'X磁相变材料
初见苗头

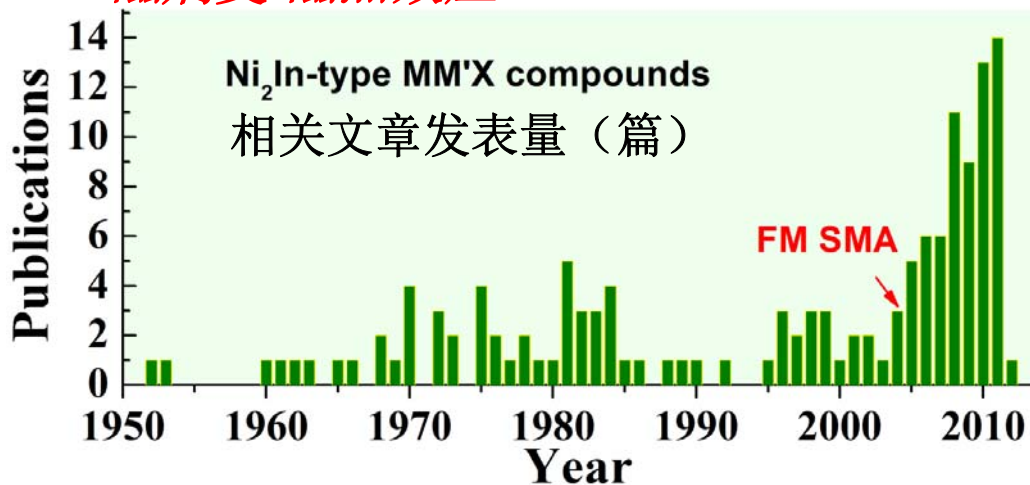


Zhang CL, et al. APL, 2008

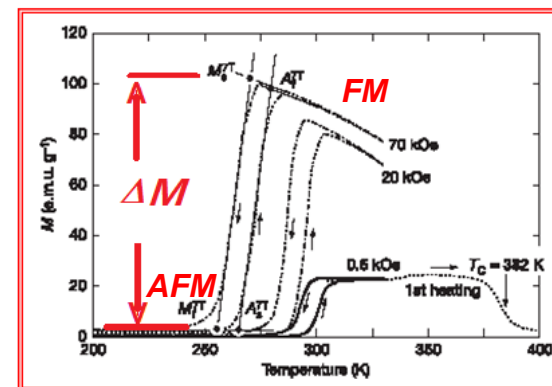
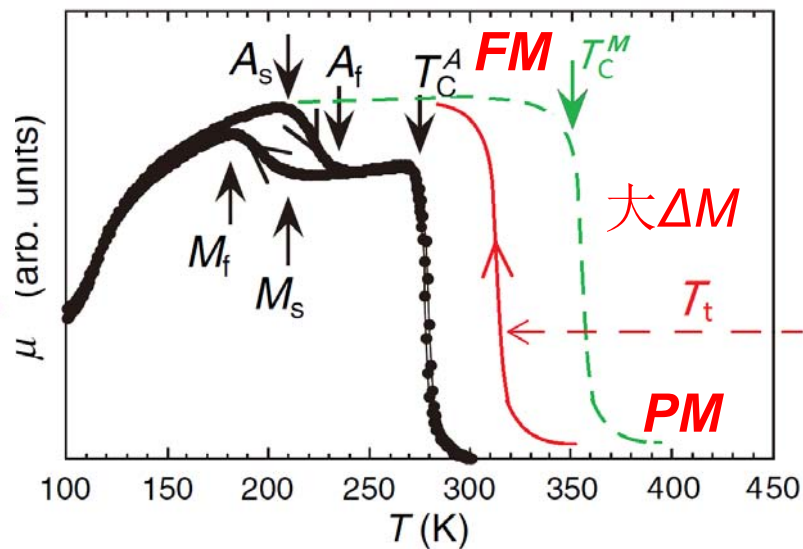
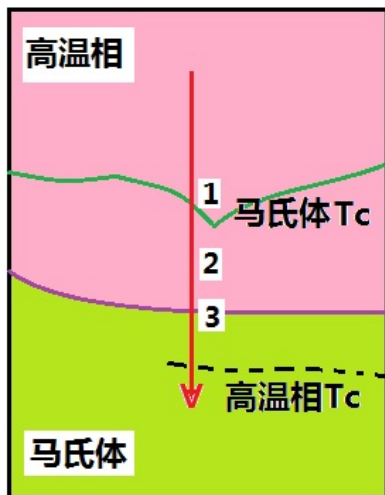
磁熵变/磁热效应



Wu GH, et al. APL, 2002

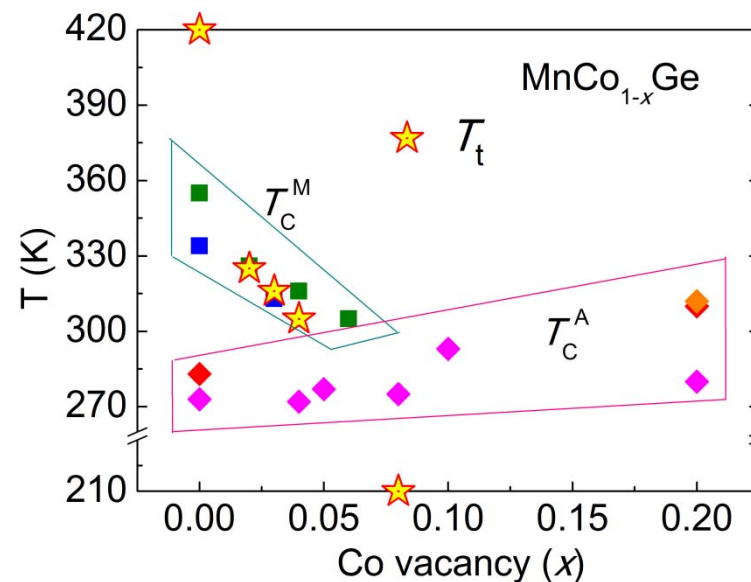
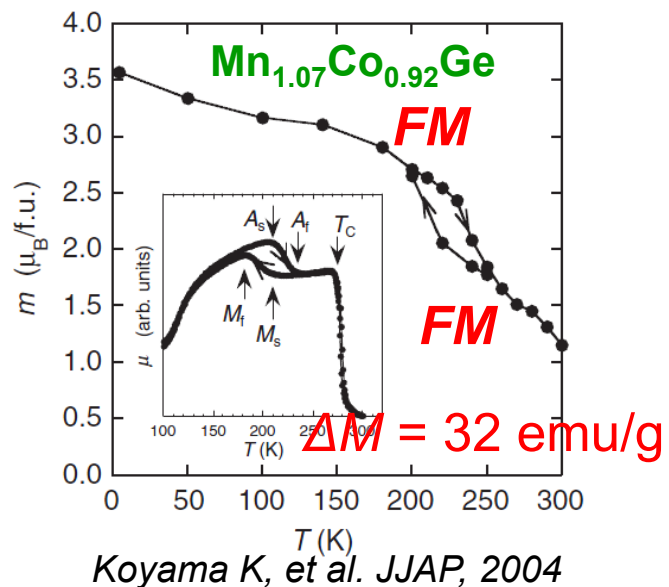


如果相变发生在温度窗口...



- ◆ 高温相低 T_c , 低温相高 T_c
- ◆ 居里温度窗口
- ◆ 相变造成可能的顺磁-铁磁转变
- ◆ 获得大 ΔM , 实现磁场驱动相变
- ◆ 相变的吸热-放热符号与磁熵变的一致

研究思路 (空位调控)



Fang, Y. K., et al.

Koyama K, et al.

Markin, P. E., et al.

◆ **Co空位导致马氏体相变温度下降**

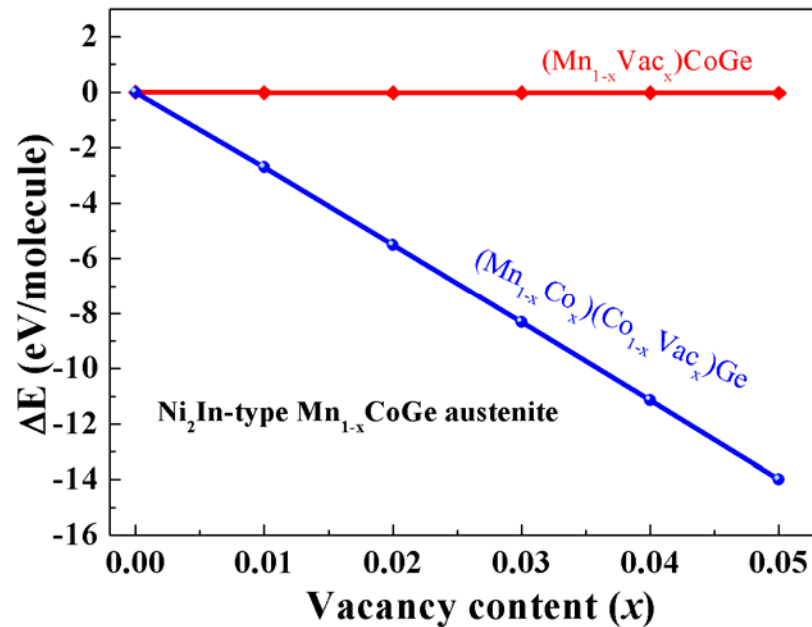
◆ **铁磁-铁磁: $\Delta M = 32 \text{ emu/g}$**

适当减少 Mn 含量会怎样?

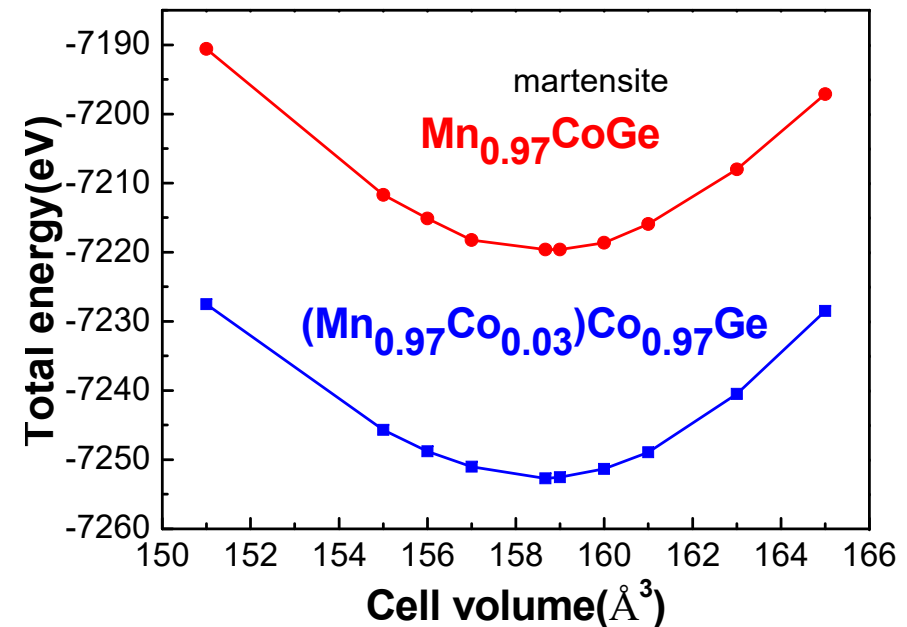
空位存在形式



高温奥氏体



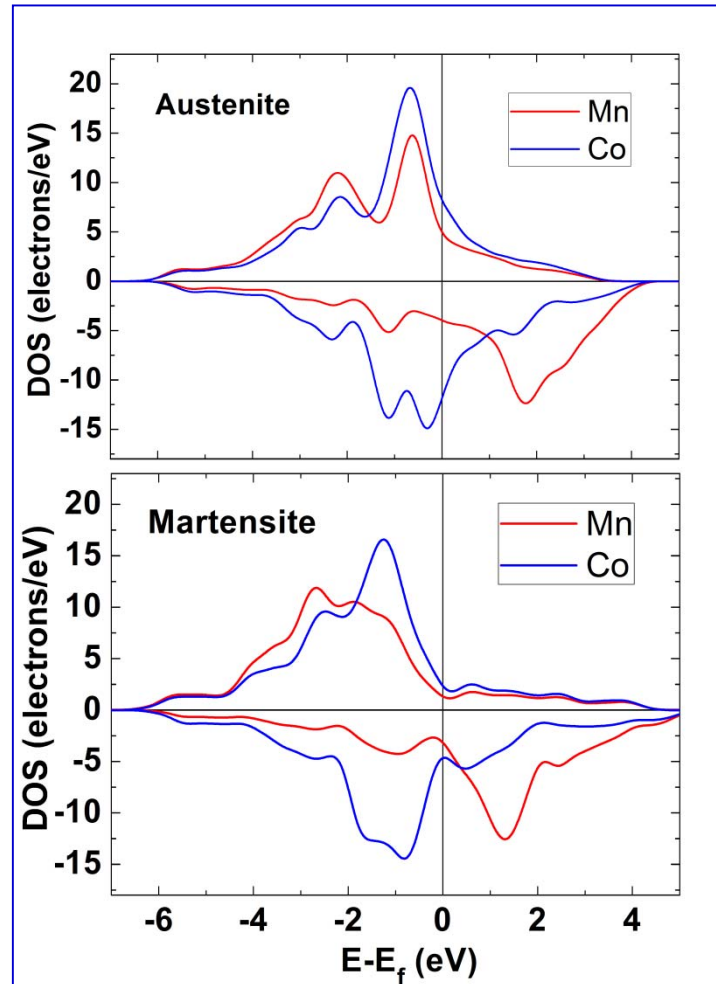
低温马氏体



计算方法:
LAPW (虚晶近似, VCA)
GGA

$(\text{Mn}_{1-x}\text{Co}_x)(\text{Co}_{1-x}\square_x)\text{Ge}$ 是 Mn-poor
 $\text{Mn}_{1-x}\text{CoGe}$ 体系的存在形式

居里温度稳定



$$T_C \propto M_0^2 / \chi_0$$

$$\chi_0^{-1} = \frac{1}{4\mu_B^2} \left[\frac{1}{N_\uparrow(\epsilon_f)} + \frac{1}{N_\downarrow(\epsilon_f)} - 2I \right]$$

Mohn, et al. *J. Phys. F: Met. Phys.* (1987)

MnCoGe	奥氏体		马氏体	
	Mn	Co	Mn	Co
自旋向上 DOS	5.00	8.22	1.32	2.35
自旋向下 DOS	3.87	11.82	3.19	4.75
原子磁矩 (μ_B)	2.68	0.50	3.04	0.70

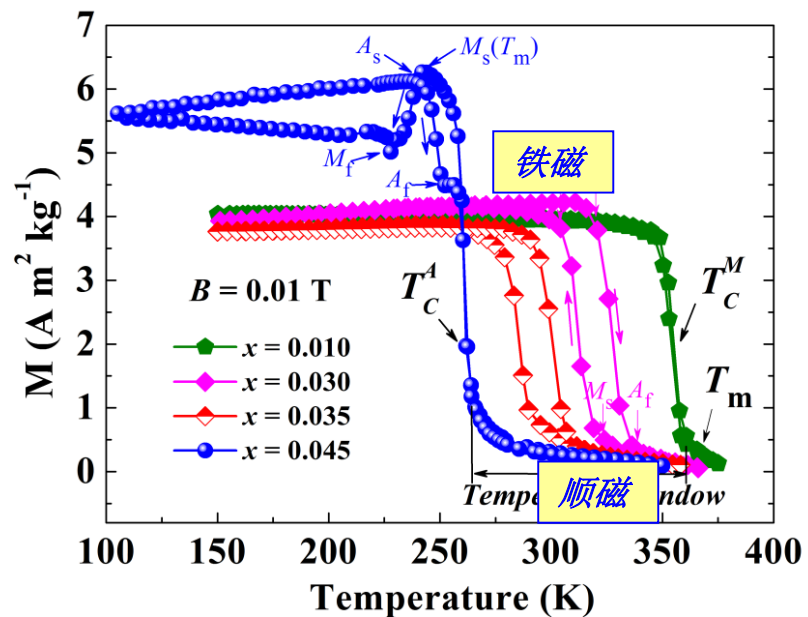
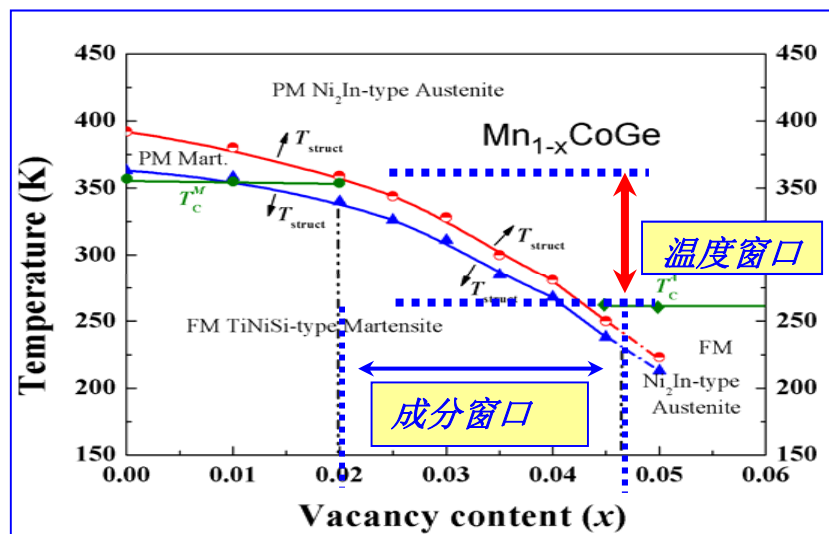
Co: 费米分布主导元素

Mn: 磁矩主要承载元素

贫Co窗口关闭，贫Mn可保持打开

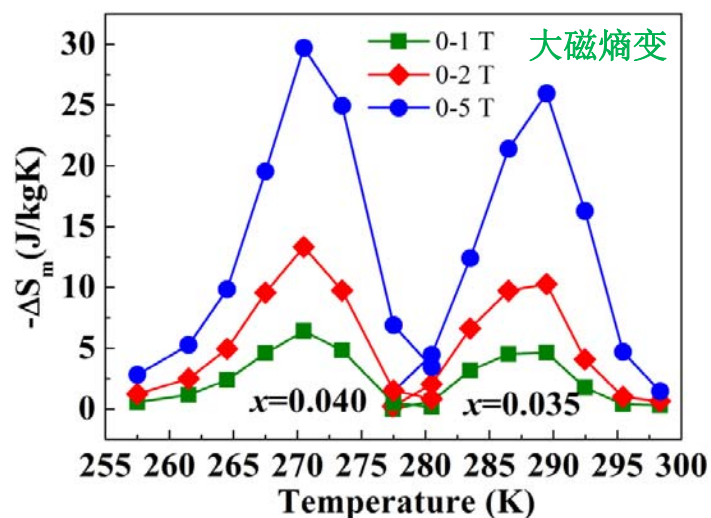
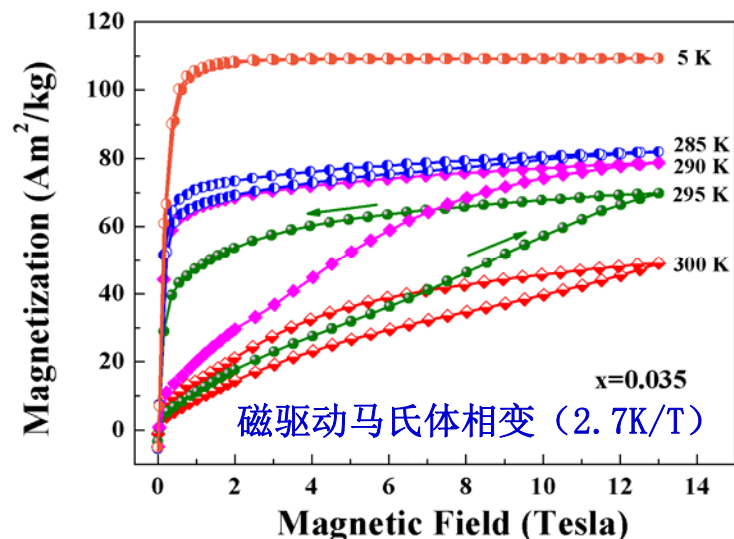
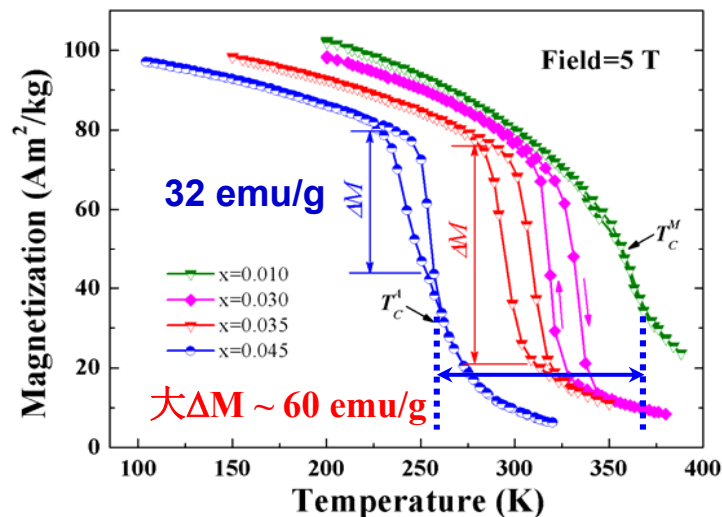
居里温度窗口

Mn_{1-x}CoGe (x=0-0.045)



- ◆ 把相变温度降到温度窗口里面
- ◆ $\Delta T \sim 90 \text{ K}$
- ◆ 空位调控相变温度

磁响应相变



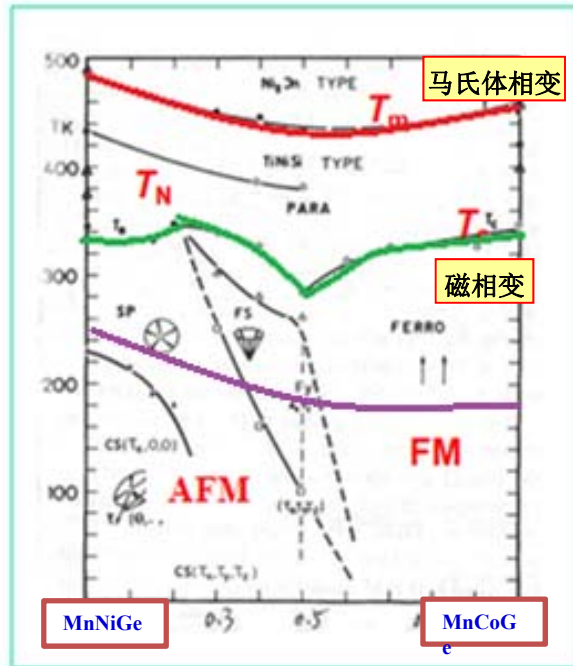
◆国际上首次报道了“温度窗口”磁驱相变, 大磁熵变

小结

主动采取居里温度窗口为调控磁驱相变的思想，在MnCoGe体系中，打开了宽约90 K的室温居里温度窗口，在其中实现了伴随有大 ΔM 的PM-FM型马氏体相变，并观察到了磁驱相变和大磁熵变。

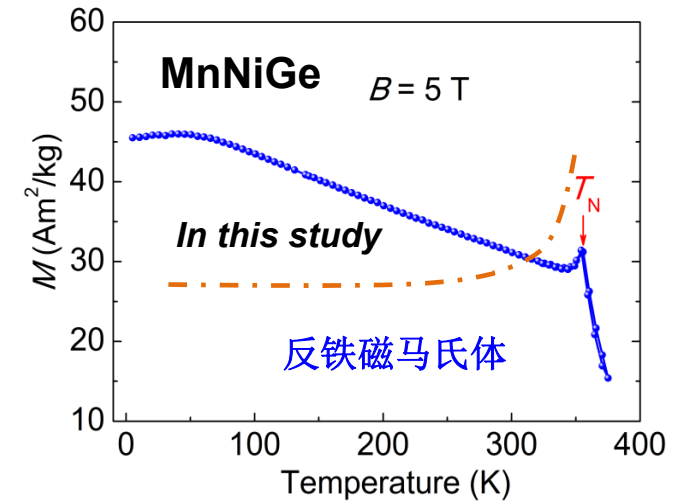
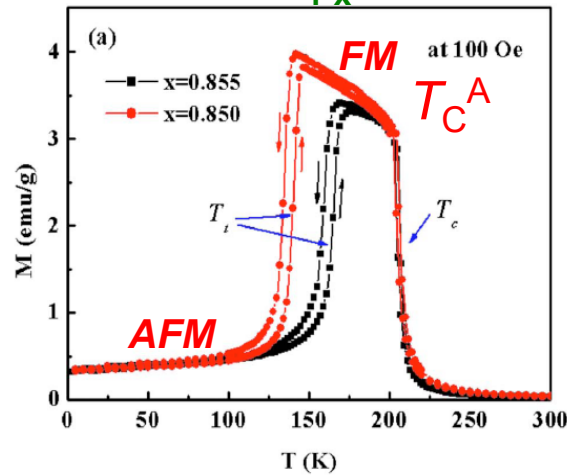
E. K. Liu, W.H.Wang and G.H.Wu et al. *Europhysics Letters* 91, 17003 (2010).

研究思路 (研究转向MnNiGe)



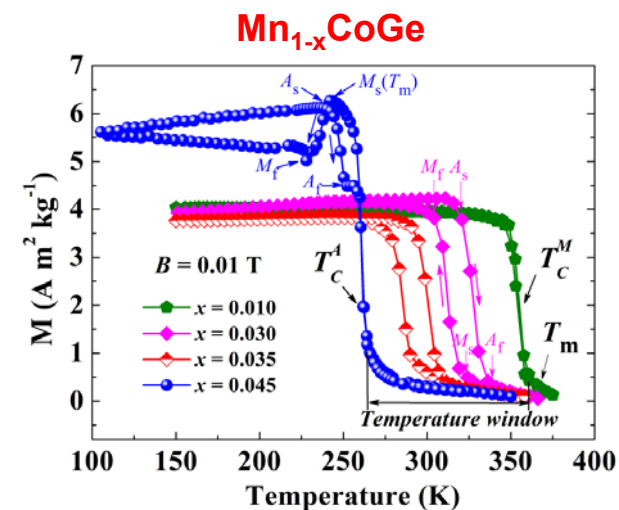
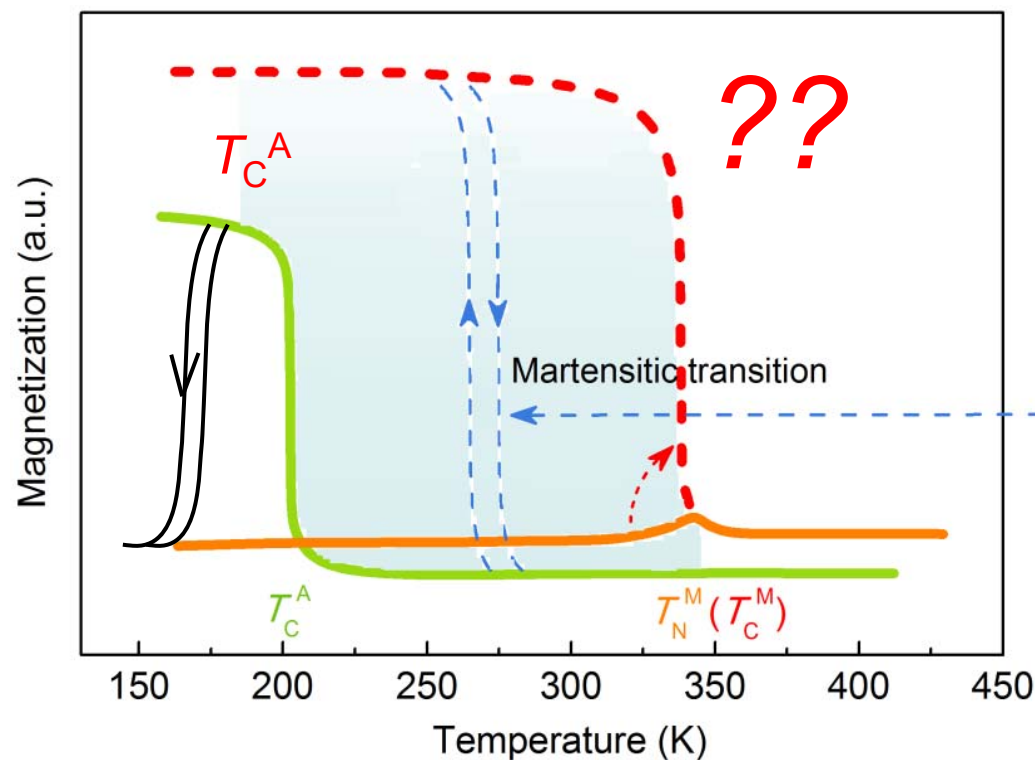
Niziol, S., et al. JMMM, 1982.

Zhang CL, et al. APL, 2008

 $\text{MnNi}_{1-x}\text{Ge}$ 

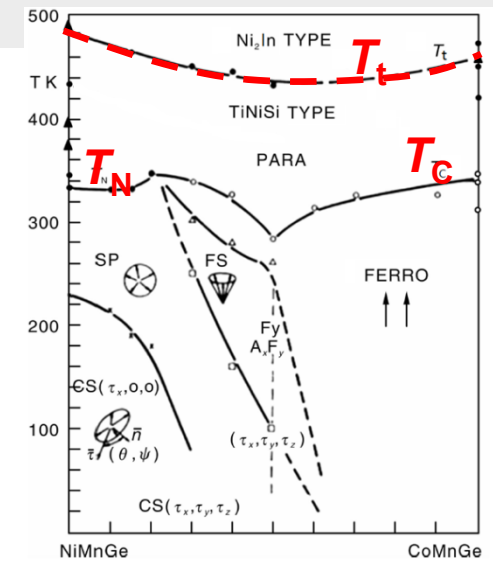
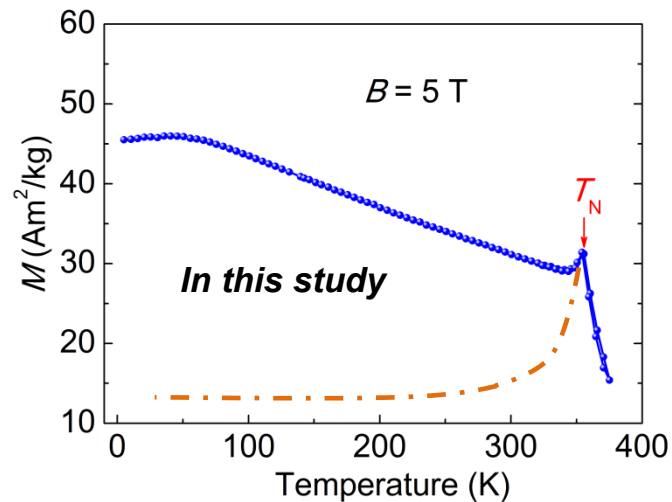
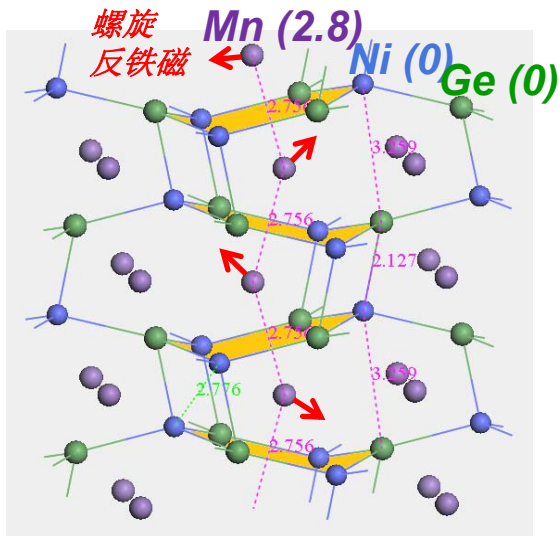
奥氏体居里温度: $T_C^A = 205 \text{ K}$
 马氏体奈尔温度: $T_N^M = 350 \text{ K}$

MnNiGe中的居里温度窗口 (两个关键问题)



1. 相变温度进窗口 (磁结构耦合, 易)
2. 马氏体反铁磁变铁磁 (大 ΔM , 难)

研究思路 磁结构调控

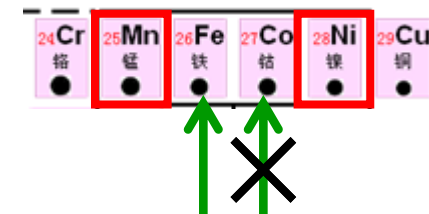


Niziol, S., et al. JMMM, 1982.

马氏体具有磁不稳定性

MnNiGe:

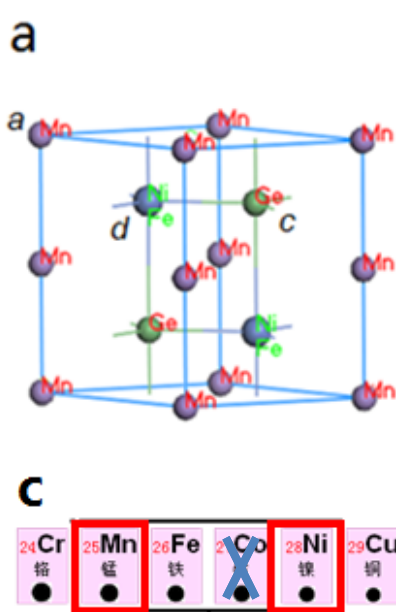
磁结构不稳定性, 易受到耦合距离、外磁场、新的FM耦合等因素的影响



降低相变温度,
引入磁性元素

研究思路 相稳定性调控

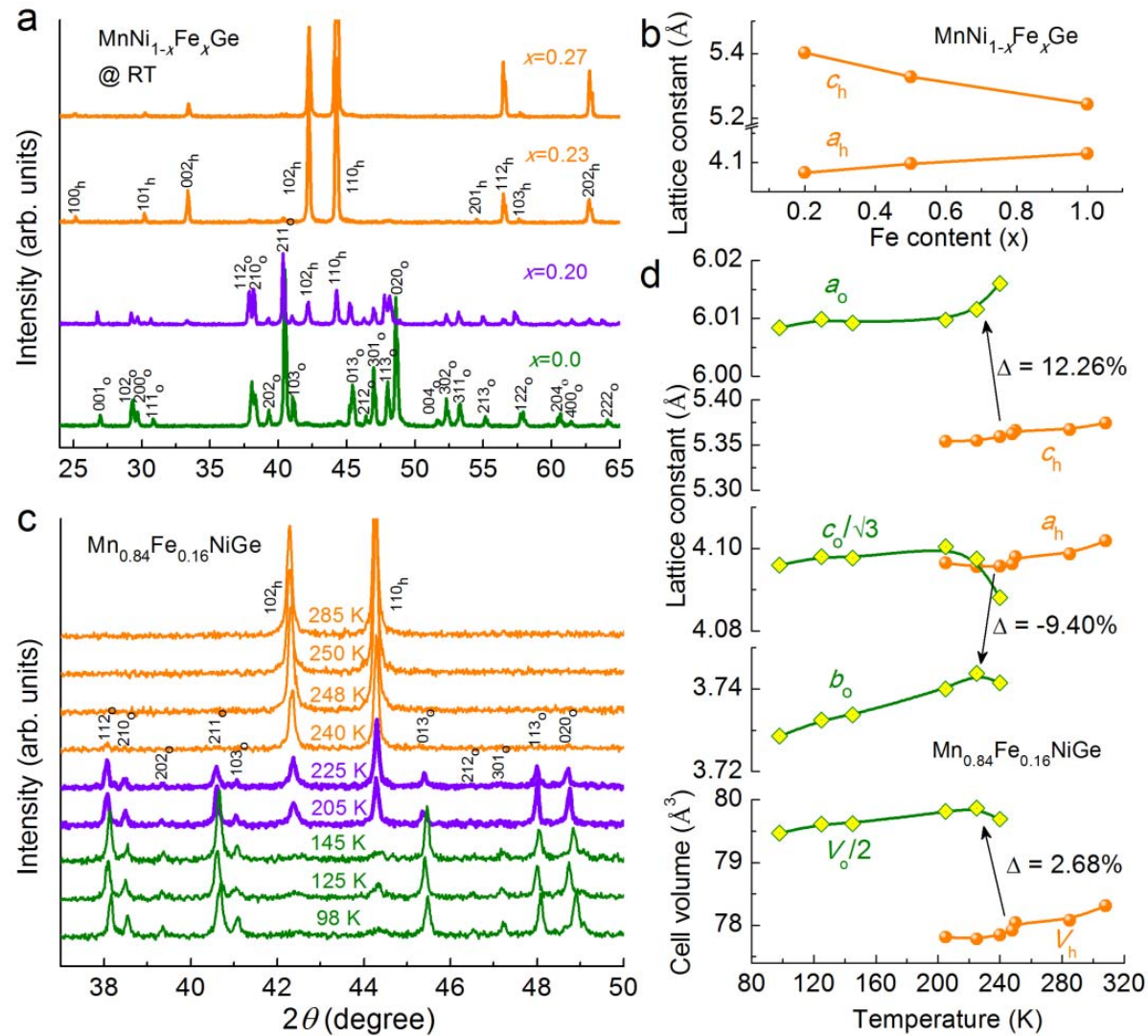
等结构合金化



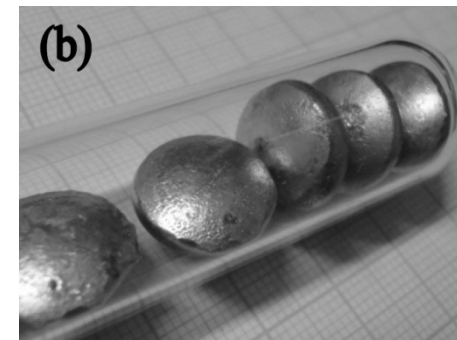
含Fe等结构体无相变

两种等结构合金化方式

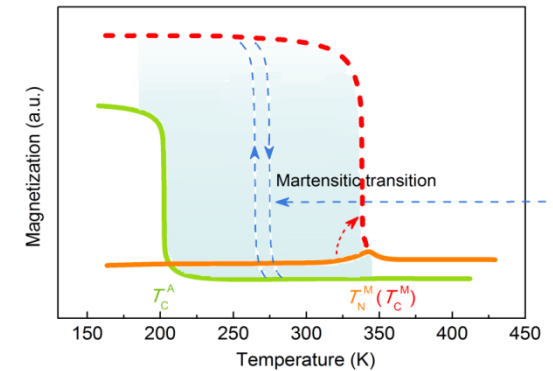
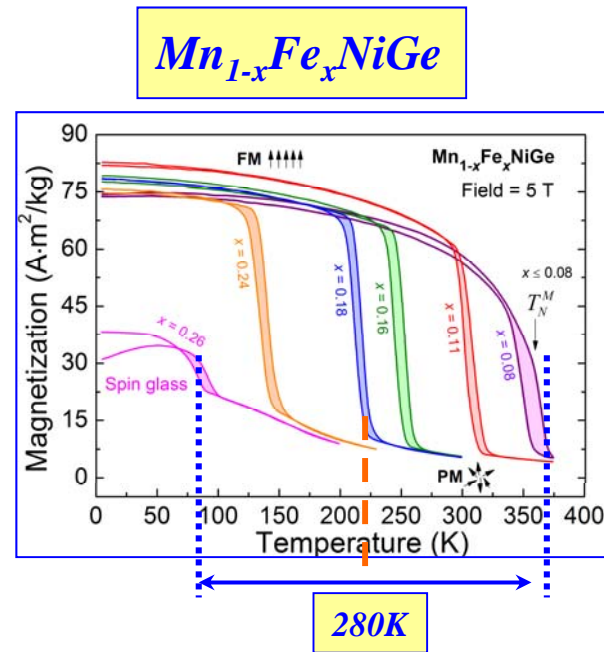
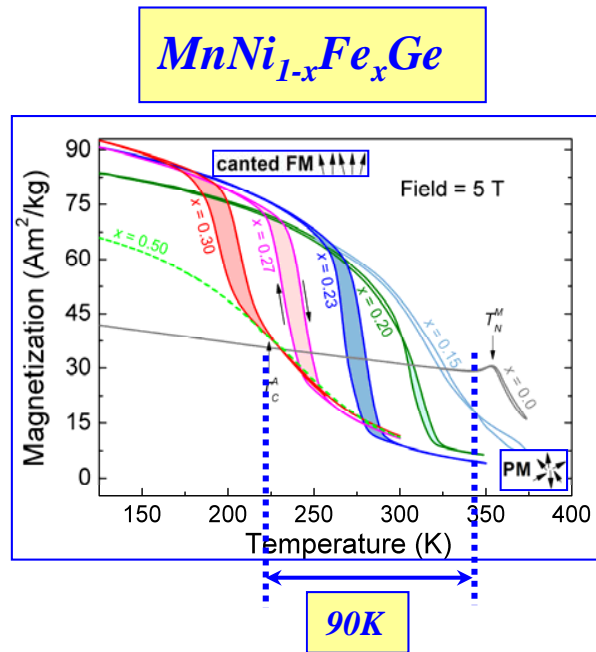
相变晶体结构



Preparation:
Arc melting (Ar atmos.);
Heat treatment:
Annealing (1123 K, 5 days, cooled slowly);
Structural analysis:
RT/T-dependent XRD;
Thermal analysis:
DTA (2.5 K/min);
Magnetic measurements:
SQUID, PPMS.

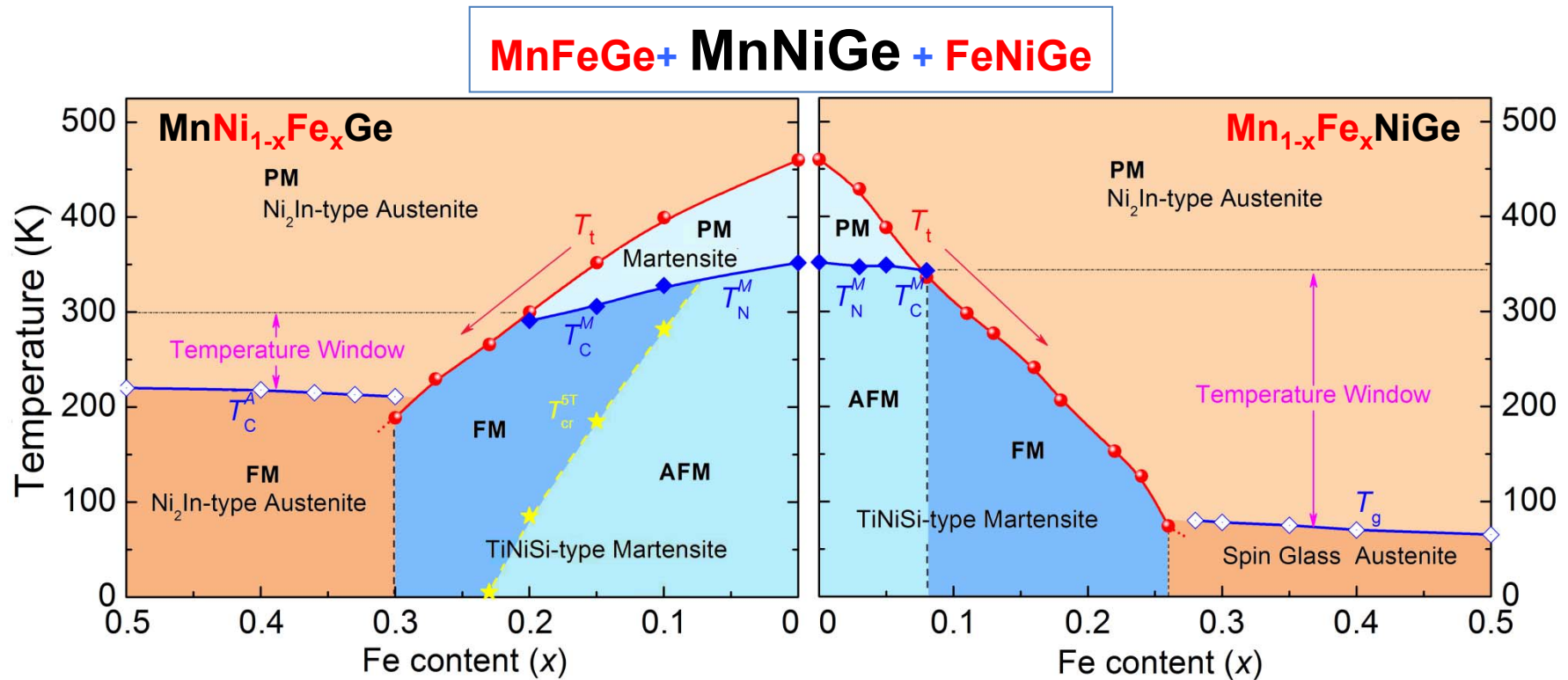


$$\begin{aligned} a_{\text{ortho}} &= c_{\text{hex}}, \\ b_{\text{ortho}} &= a_{\text{hex}}, \\ c_{\text{ortho}} &= \sqrt{3}a_{\text{hex}}, \\ V_{\text{ortho}} &= 2V_{\text{hex}} \end{aligned}$$



- ◆ MnFeGe, FeNiGe 都没有相变，确实起到降低 T_t 的作用
- ◆ 而Fe 取代Ni和Mn在马氏体中都可以实现AFM-FM转变
- ◆ FeNiGe 的高温相是顺磁的，降低了高温相的 T_c ，将窗口拓宽一倍（室温以上-液氮温度）

磁性及结构相图



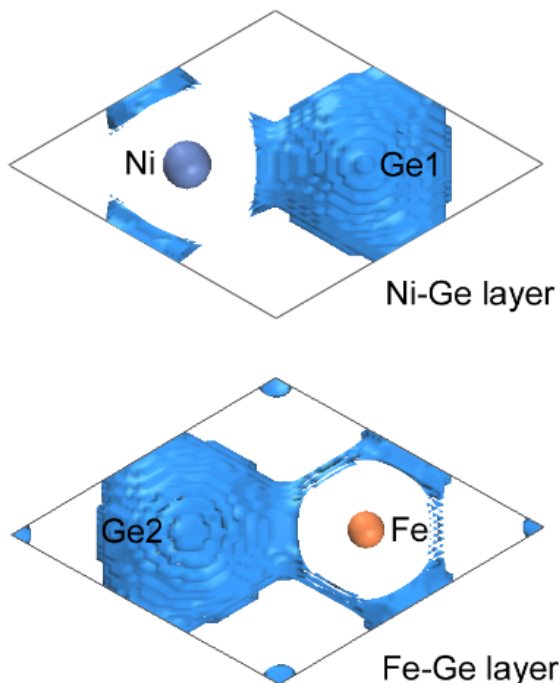
Temperature window: 90 K \longrightarrow 扩展至280 K

<300 ~ 210 K>

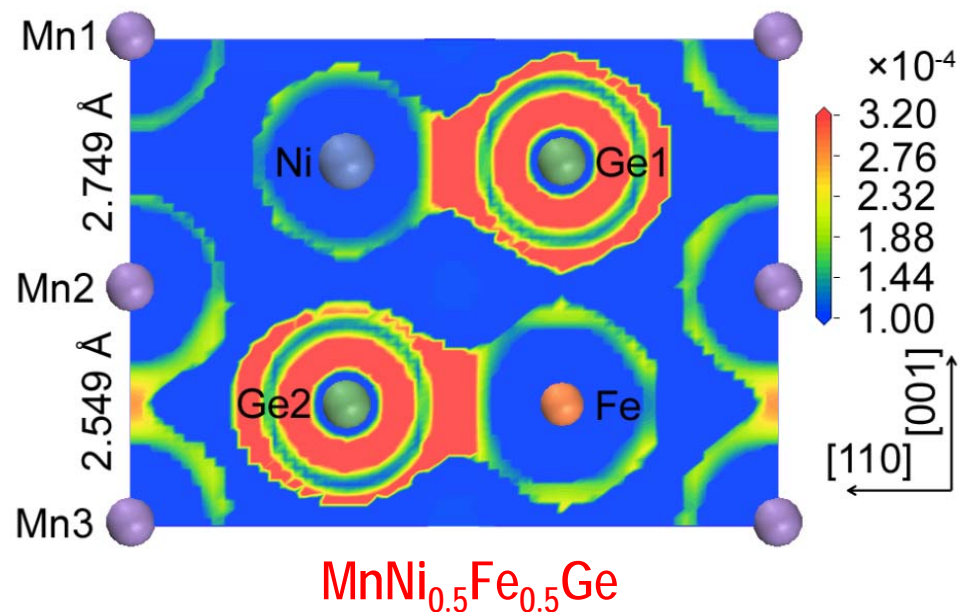
<350 ~ 70 K>

相稳定性调控机理 相变温度为什么会降低？

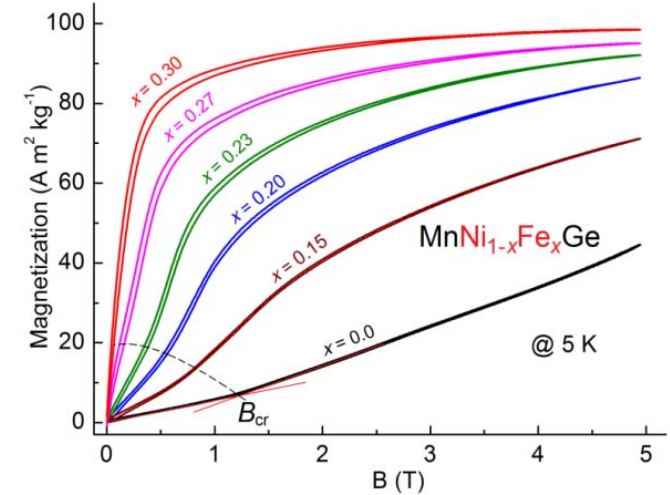
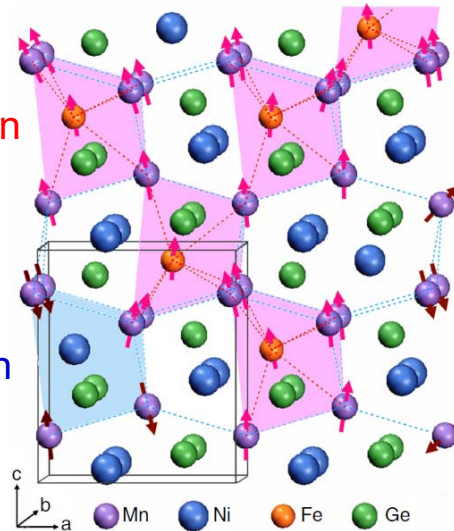
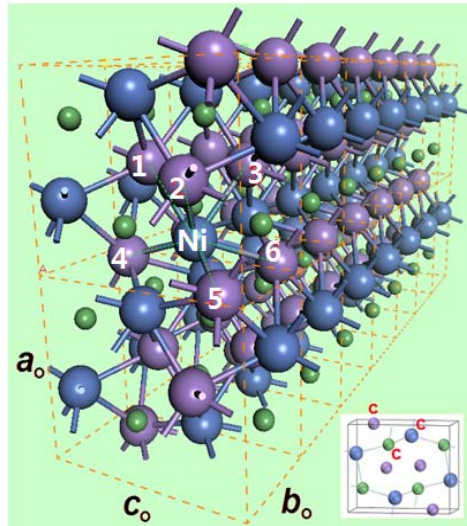
电子定域函数计算



Pseudopotential method,
plane-wave-basis set,
LSDA, cut-off energy 770 eV,
k points $13 \times 13 \times 12$,

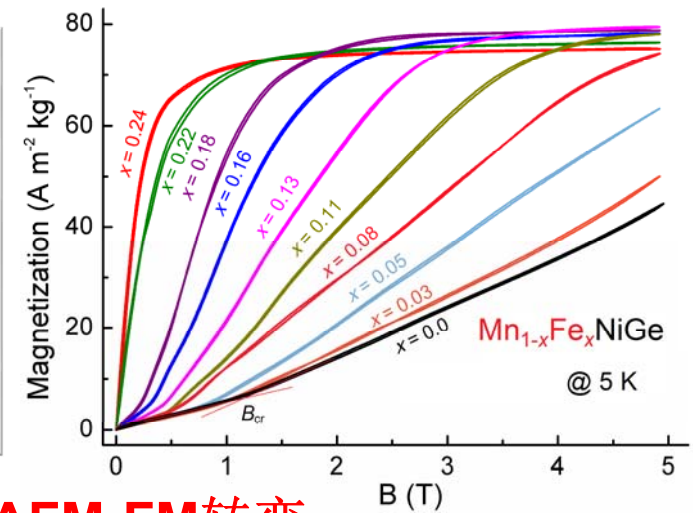


- ◆ 将MnNiGe 和 MnFeGe 等结构合金化 (Fe 取代 Ni)
- ◆ Fe-Ge、Mn-Mn共价作用增强，母相稳定化，相变温度降低

磁结构调控机理 原子配置分析 ($\text{MnNi}_{1-x}\text{Fe}_x\text{Ge}$)

原子	间距 (Å)
Mn-Mn	3.2
Mn-Ni	2.8
Mn-Fe	2.8
Ni-Ge	2.4
Fe-Ge	2.3

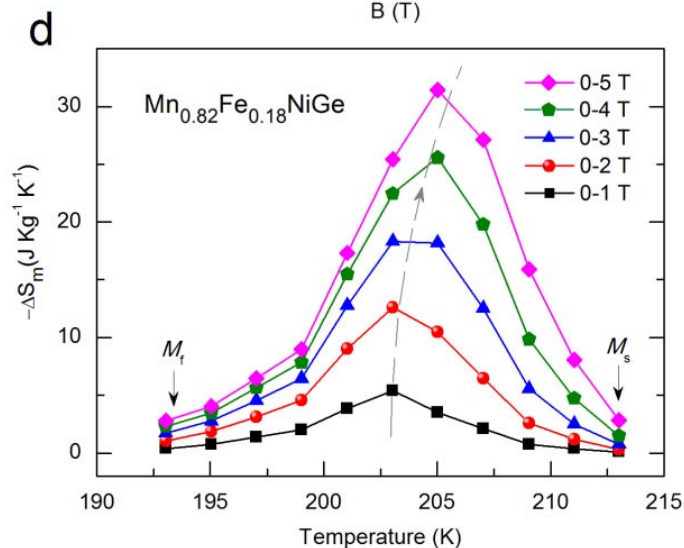
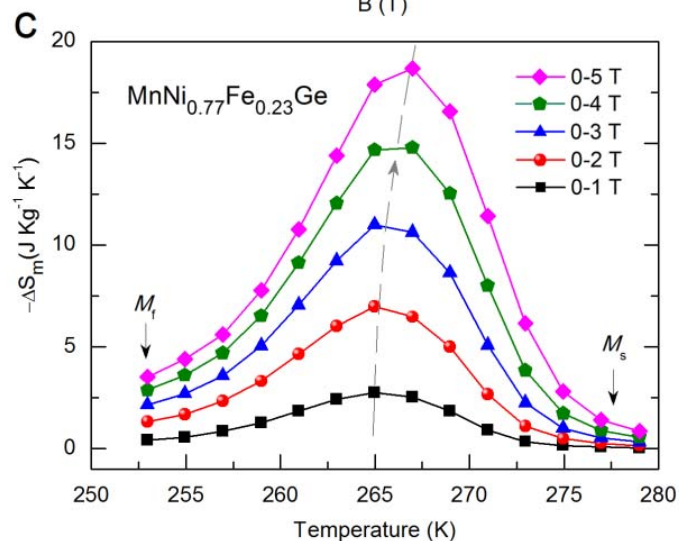
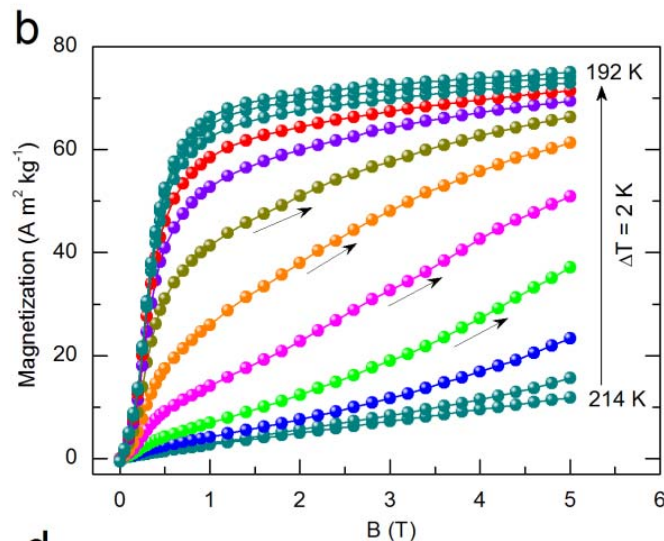
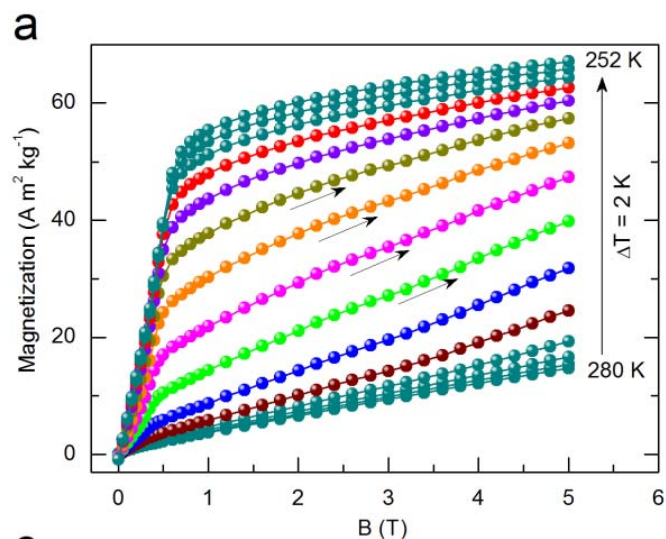
	理论计算	实验测量
Mn	2.8-2.9	
Ni	0.08-0.2	
Fe	1.44	$\text{MnNi}_{0.25}\text{Fe}_{0.25}\text{Ge}$
Ge	-0.02	
分子磁矩	3.33	3.11



马氏体相AFM-FM转变

磁驱相变及大磁熵变

LOOP Process Method



Gd₅Si₂Ge₂
(2 T : -14 J/kg K)

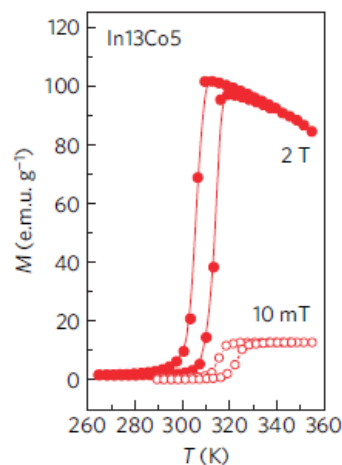
Ni₅₀Mn₃₇Sn₁₃
(5 T : 18 J/kg K)

MnFeP_{0.45}As_{0.55}
(5 T : -18 J/kg K)

LaFe_{11.4}Si_{1.6}
(5 T : -20 J/kg K)

非稀土Mn基
可调大磁熵变

一致的热效应

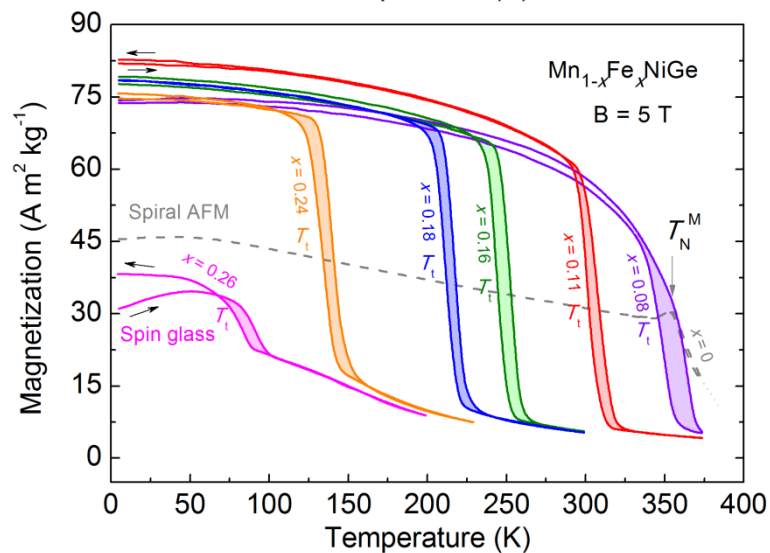
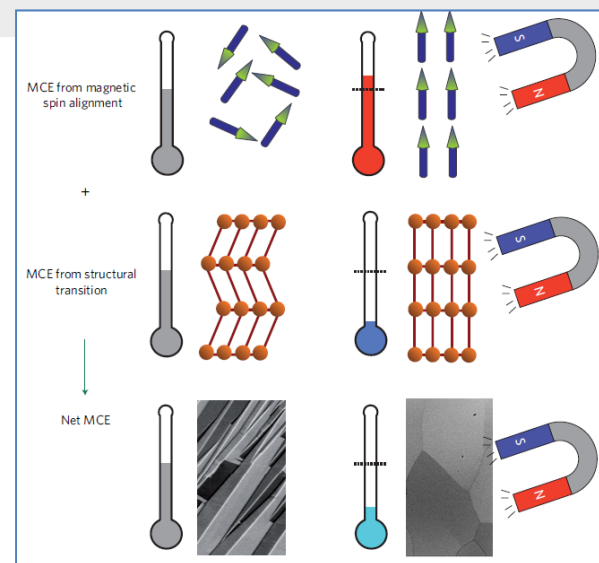


Jian Liu, et al., *Nature Materials*, 2012

Heusler alloy
 $Ni_{45.2}Mn_{36.7}In_{13}Co_{5.1}$



磁场诱发逆马氏体相变



E.K. Liu, W.H. Wang and G.H.Wu. et al., *Nature Communications*, 3, 873, 2012

1. **Stable magnetostructural coupling with tunable magnetoresponse effects in hexagonal ferromagnets**

作者: Liu, Enke; Wang, Wenhong; Feng, Lin; 等.

NATURE COMMUNICATIONS 卷: 3 文献号: 873 出版年: MAY 2012

Context Sensitive

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排序方式:

出版日期 (降序)

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来自 *Essential Science Indicators* 的数据

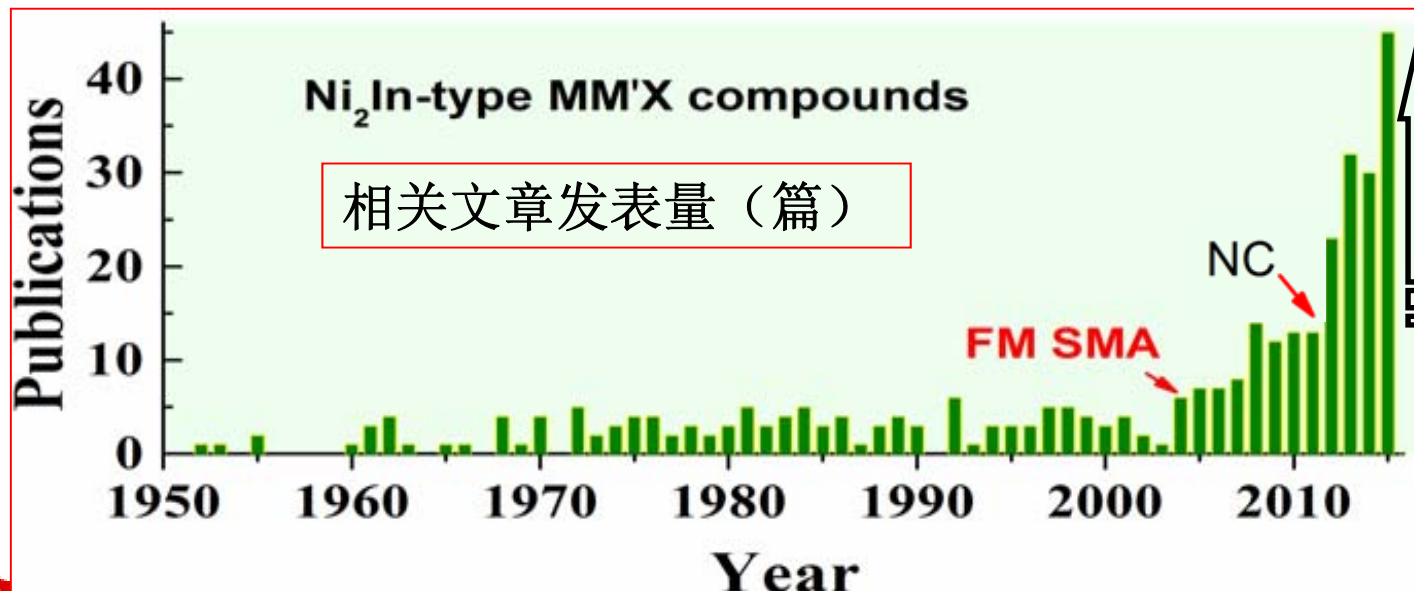
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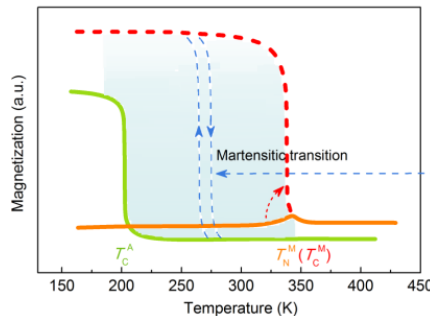
文章发表量
增加 4 倍

国际 40 多个
课题组

小结

以居里温度窗口作为调控磁驱动马氏体相变的思路，采用单一而有效的等结构合金化方法，同步实现了材料设计的多个目标，获得了具有优异性能的新型铁磁马氏体相变材料。

在 $\text{MnNi}_{1-x}\text{Fe}_x\text{Ge}$ 和 $\text{Mn}_{1-x}\text{Fe}_x\text{NiGe}$ 体系分别获得了宽约**90 K**和**280 K**的大居里温度窗口，实现了**PM-FM型**马氏体相变，观察到了显著的**磁驱动马氏体相变**和**巨磁热效应**。)

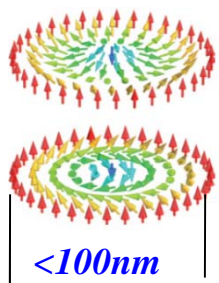


事实证明，传统材料里面确有新东西

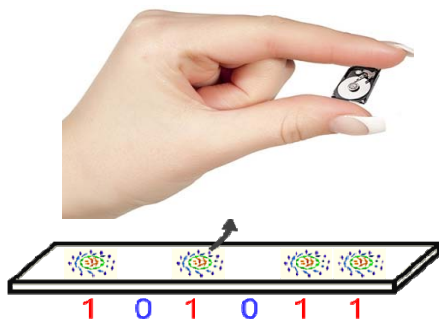
E. K. Liu, W.H.Wang and G.H.Wu et al. *Nature Communications*, 3, 873, 2012

磁性斯格明子 最小的拓扑纳米磁结构

Tony Skyrme 1962

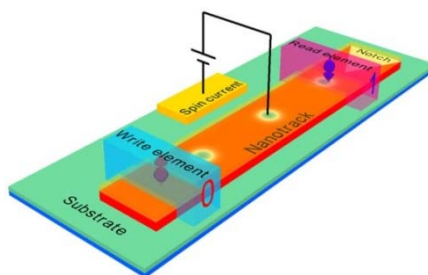


磁信息存储



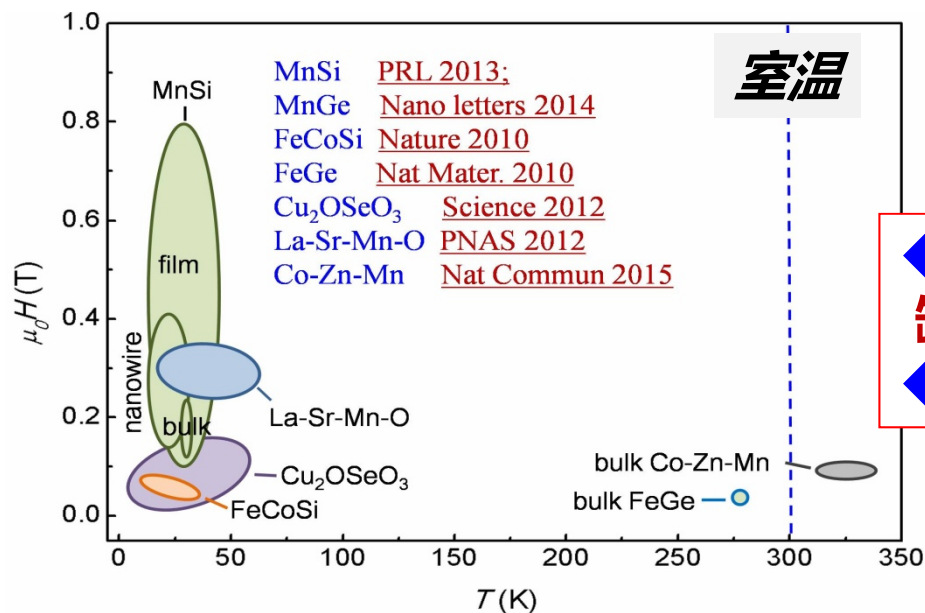
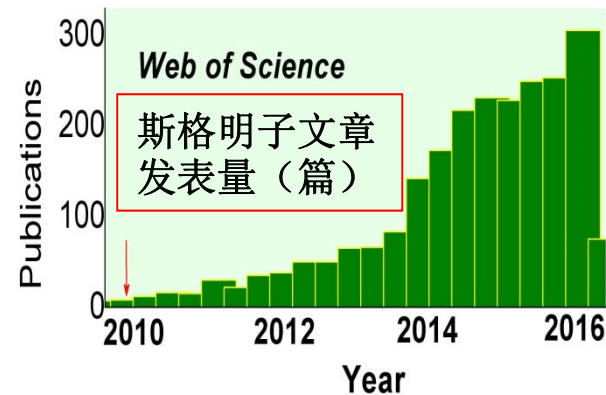
X. Z. Yu et al., Nature (2010)

自旋电子学器件



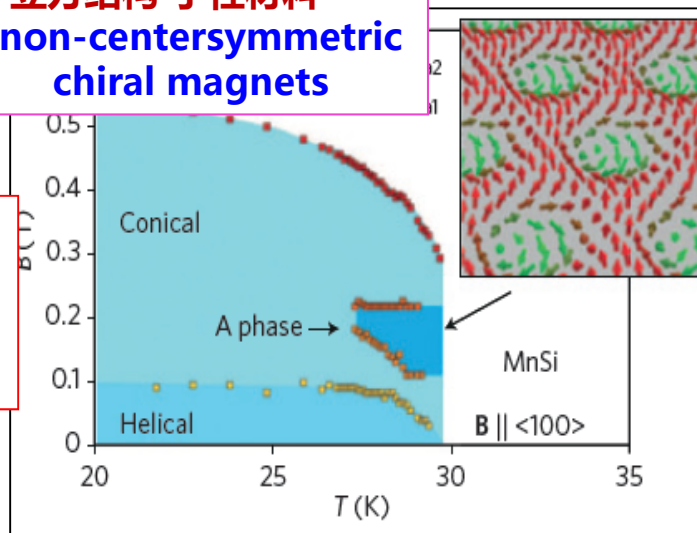
F. Jonietz et al., Science (2010)

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立方结构 手性材料
Cubic non-centersymmetric chiral magnets

◆低温
缺点：
◆温区窄



提高磁斯格明子稳定性

-纳米线

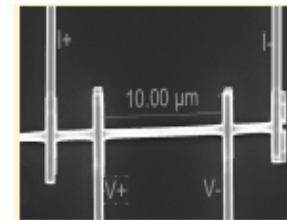
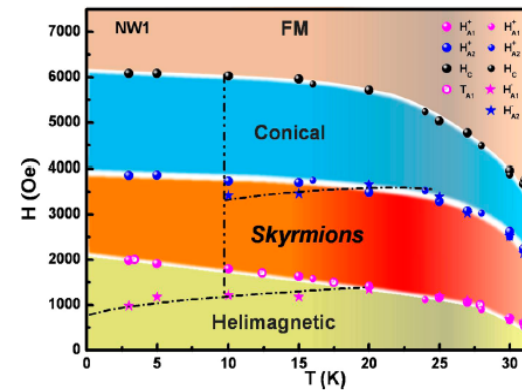
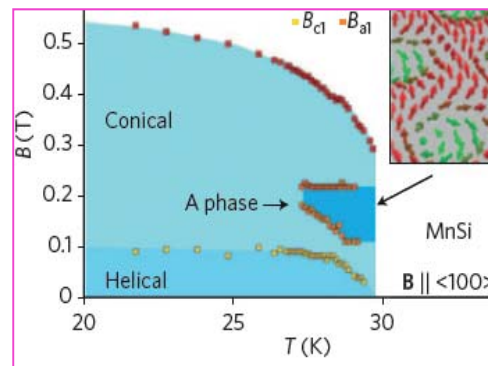
NANO LETTERS

Letter

pubs.acs.org/NanoLett

Highly Stable Skyrmion State in Helimagnetic MnSi Nanowires

Haifeng Du,^{1,2} John P. DeGrave,³ Fei Xue,^{1,2} Dong Liang,³ Wei Ning,^{1,2} Jiyong Yang,^{1,2}
Mingliang Tian,^{4,5,6} Yuheng Zhang,^{1,2} and Song Jin^{4,5,6}



26~30K in bulk



10~ 35K in nanowires

提高磁斯格明子稳定性

-薄膜

PRL 108, 267201 (2012)

PHYSICAL REVIEW LETTERS

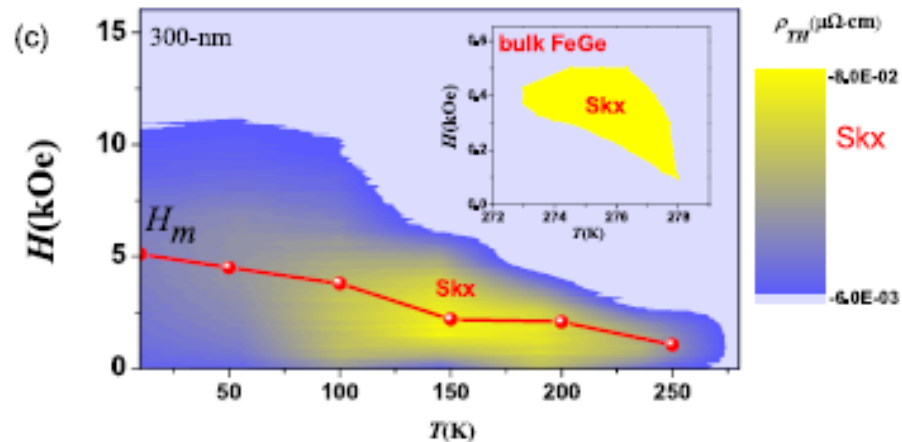
week ending
29 JUNE 2012

Extended Skyrmion Phase in Epitaxial FeGe(111) Thin Films

S. X. Huang* and C. L. Chien†

Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, Maryland 21218, USA

(Received 4 April 2012; published 26 June 2012)



273~278K in bulk



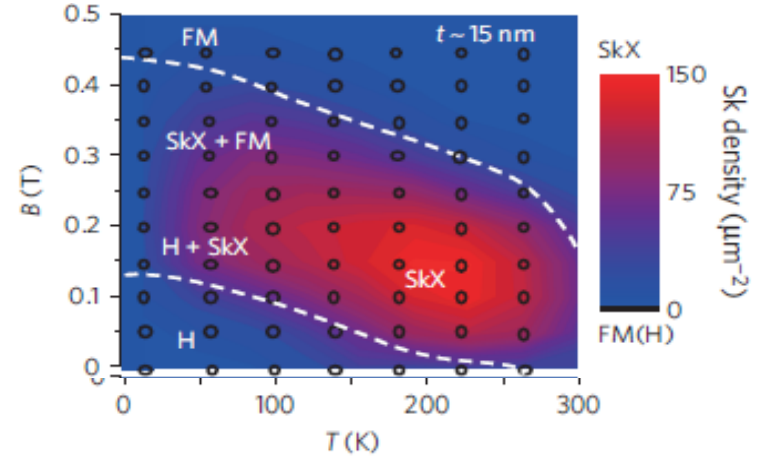
50~280K in thin films

LETTERS

PUBLISHED ONLINE 5 DECEMBER 2010 | DOI: 10.1038/NMAT2916

nature
materials

Near room-temperature formation of a skyrmion crystal in thin-films of the helimagnet FeGe

X. Z. Yu^{1*}, N. Kanazawa², Y. Onose^{1,2}, K. Kimoto³, W. Z. Zhang³, S. Ishiwata², Y. Matsui³ and Y. Tokura^{1,2,4*}

提高磁斯格明子稳定性

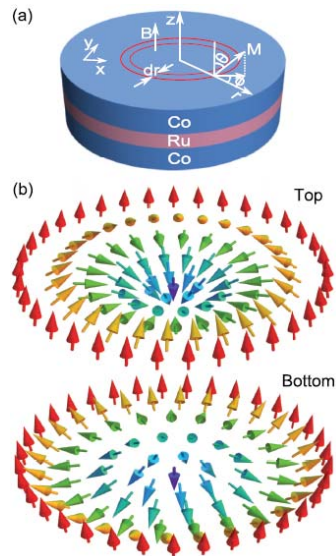
-patterned nanodisks

PHYSICAL REVIEW B 88, 054403 (2013)

Skyrmion ground state and gyration of skyrmions in magnetic nanodisks without the Dzyaloshinsky-Moriya interaction

Y. Y. Dai,^{*} H. Wang,^{*} P. Tao, T. Yang, W. J. Ren, and Z. D. Zhang[†]

Shenyang National Laboratory for Materials Science, Institute of Metal Research and International Centre for Materials Physics, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, People's Republic of China

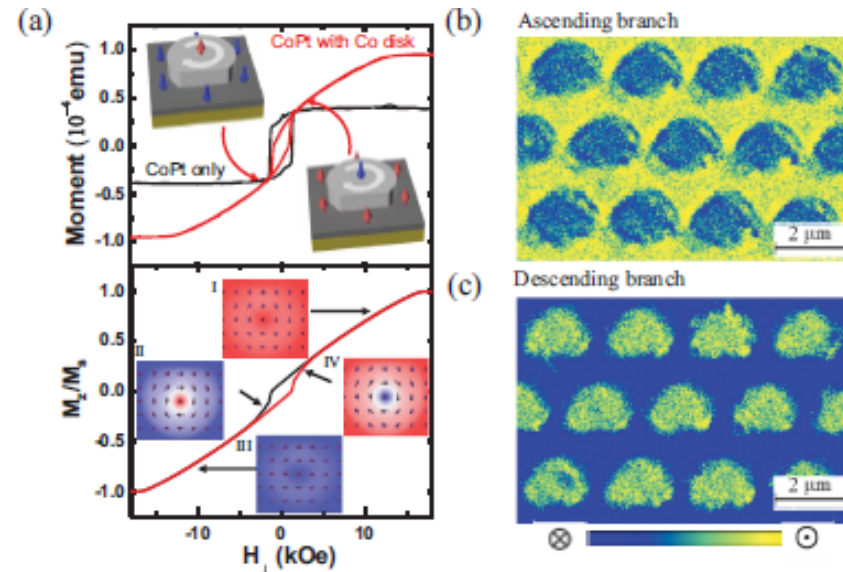


不考虑DMI

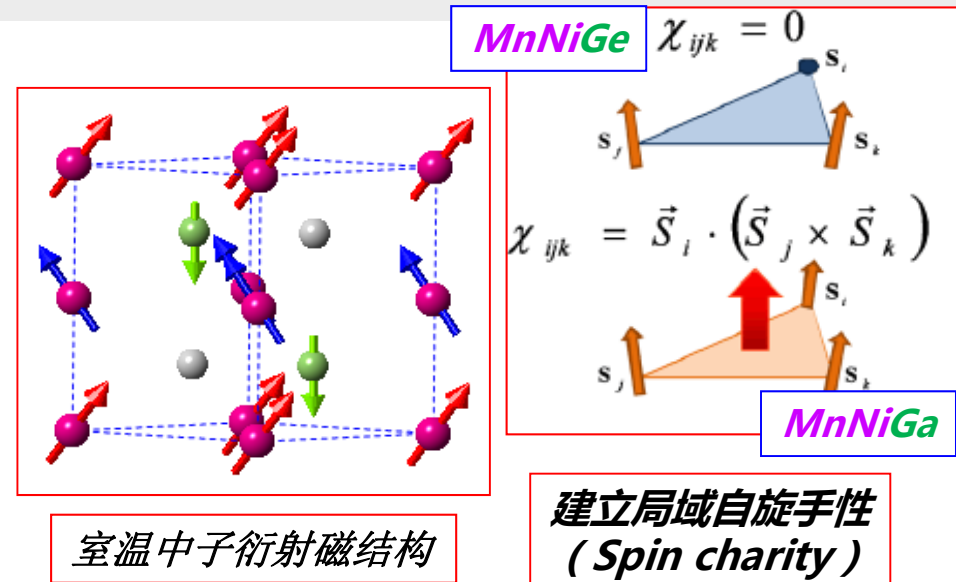
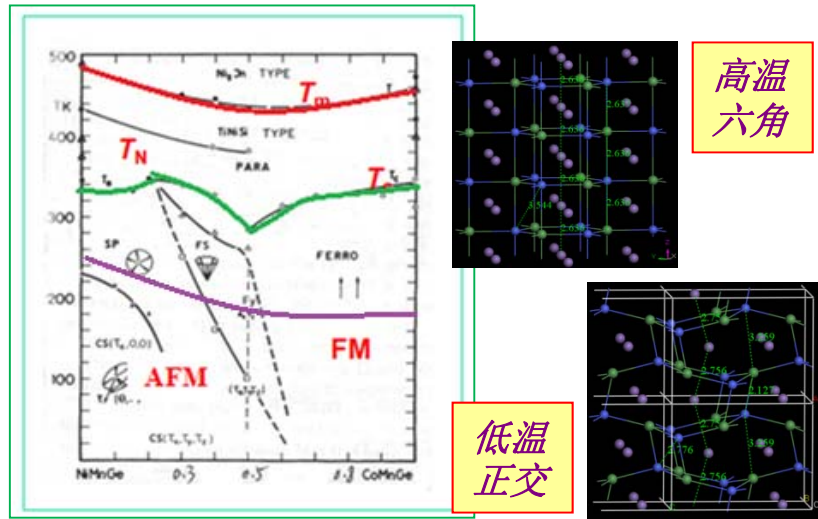
考虑：交换能、磁晶各向异性能和退磁能之间的竞争

PHYSICAL REVIEW B 90, 174411 (2014)

Experimental realization of two-dimensional artificial skyrmion crystals at room temperature

B. F. Miao,¹ L. Sun,¹ Y. W. Wu,¹ X. D. Tao,¹ X. Xiong,¹ Y. Wen,¹ R. X. Cao,¹ P. Wang,¹ D. Wu,¹ Q. F. Zhan,² B. You,¹ J. Du,¹ R. W. Li,² and H. F. Ding^{1,*}

斯格明子形成基本条件：**高对称性+非共线磁+手性**

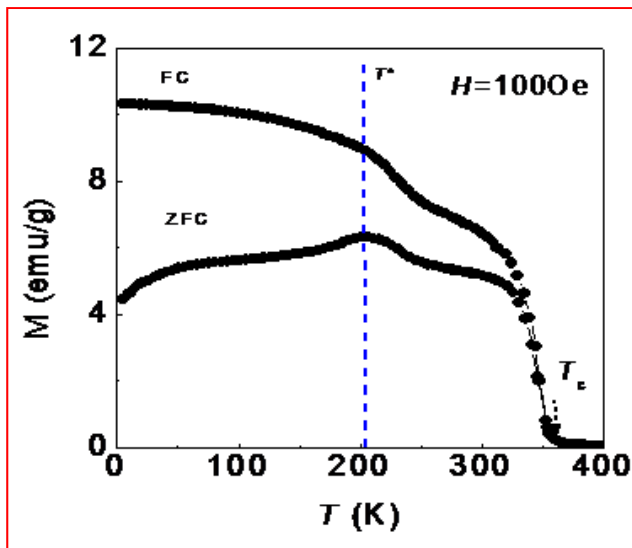


室温中子衍射磁结构

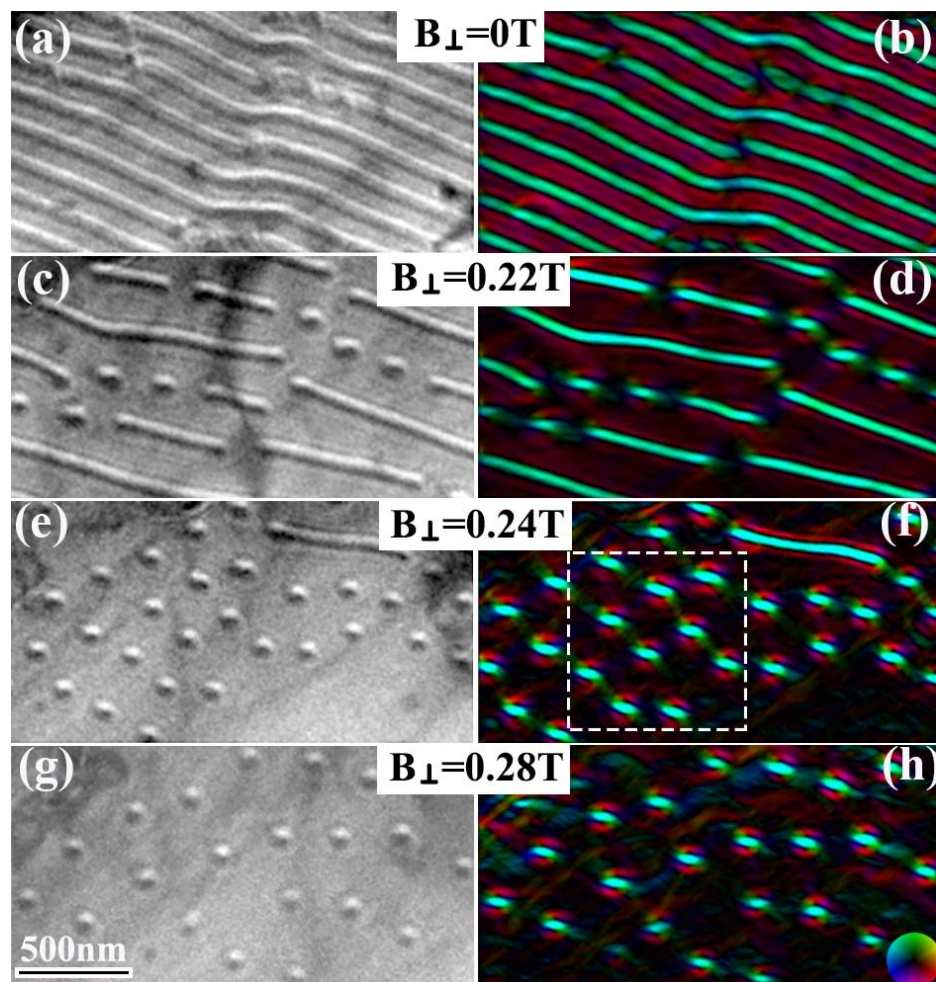
Ga替代Ge

- ◆ 结构相变压制，磁相变发生
- ◆ 建立局域自旋手性

六角MnNiGa满足skymion形成条件



洛伦兹电镜：磁场诱发磁斯格明子的直接观察



Magnetic helical spin structure @ 0T

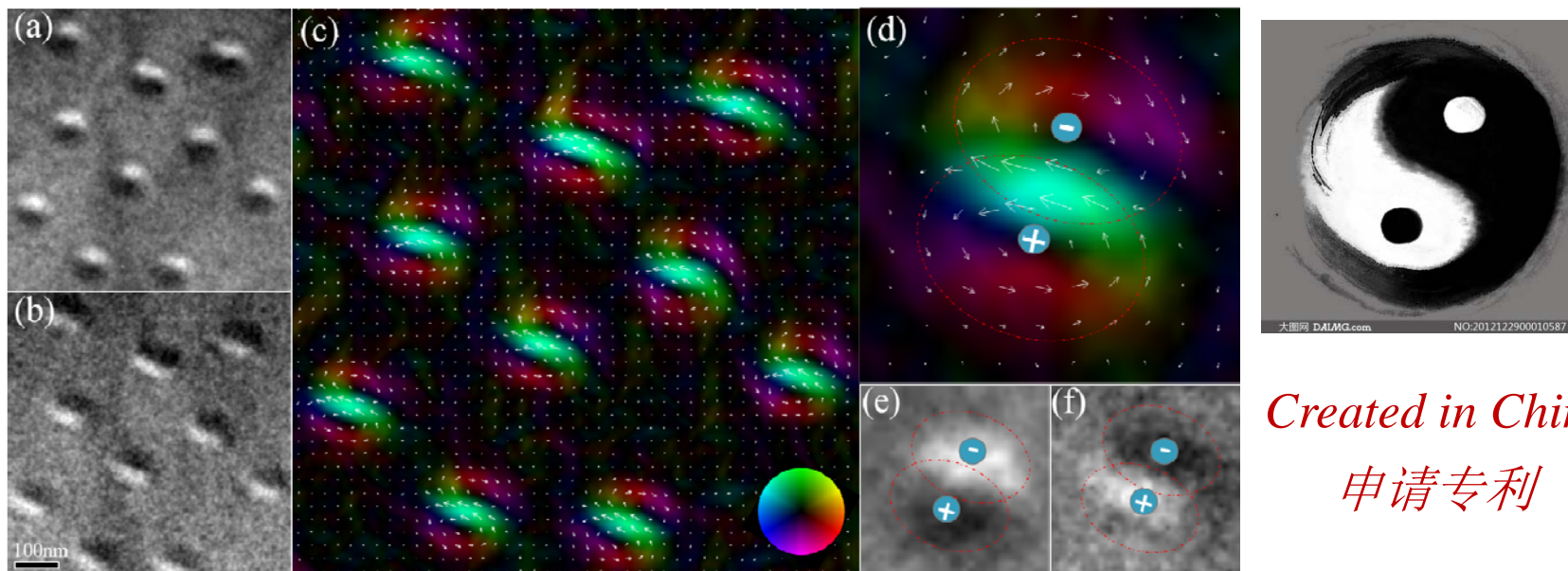


Helical + Skyrmion spin structure @ 0.22T



Skyrmion spin structure @ $B > 0.28T$

磁斯格明子的拓扑自旋结构



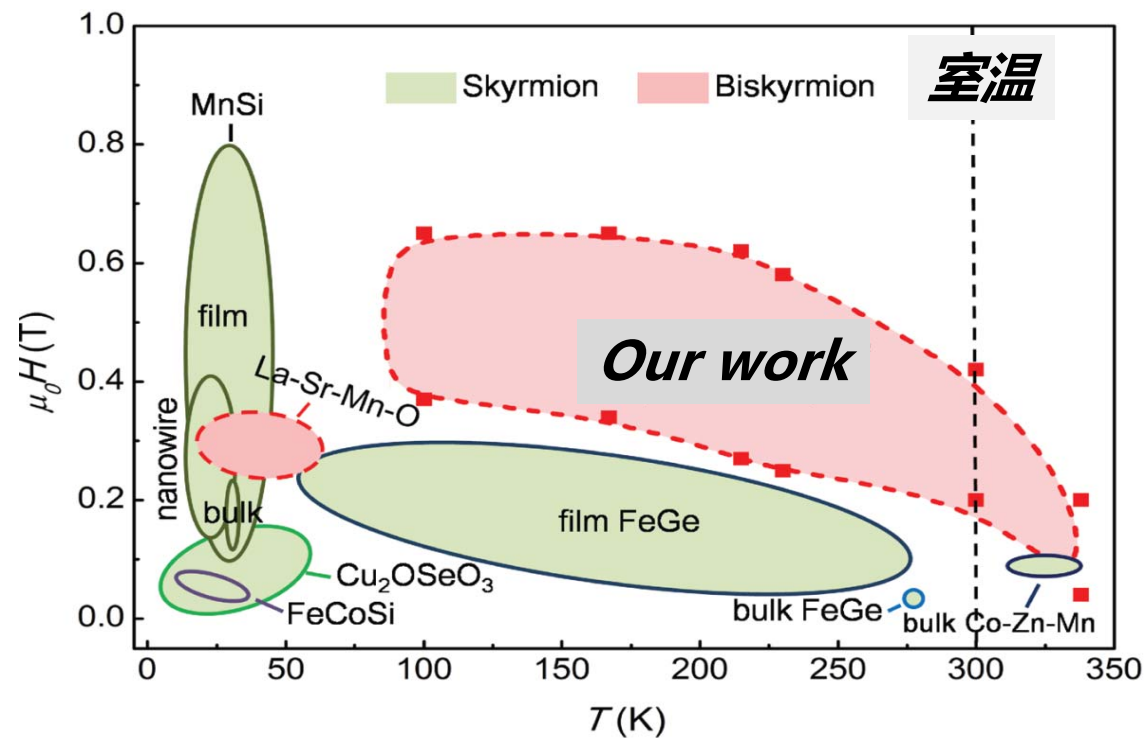
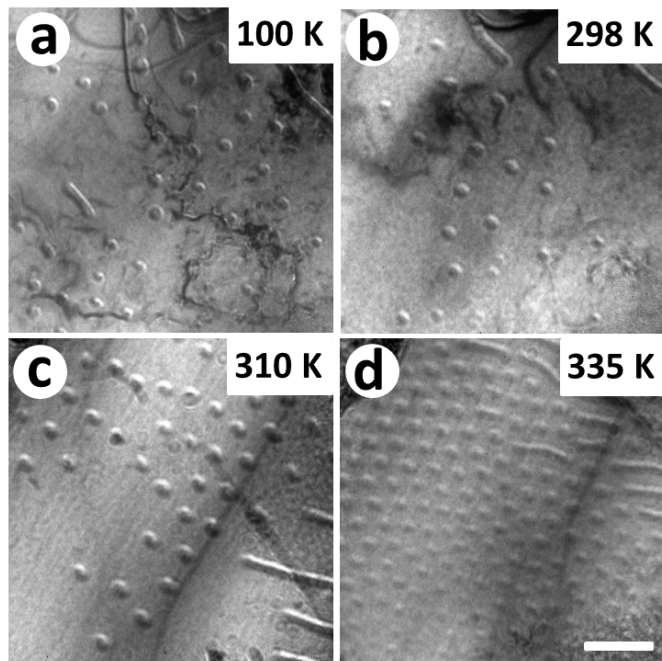
Created in China

申请专利

- ◆ *Biskyrmion spin texture $\sim 90\text{nm}$*
- ◆ *Topological number $N=2$*

Biskyrmions 不同于之前DM相互作用的skymions 磁结构

磁斯格明子稳定性：宽温区，跨室温，强磁性



W.H.Wang, et al., Adv. Mater. 2016

A Centrosymmetric Hexagonal Magnet with Superstable Biskyrmion Magnetic Nanodomains in a Wide Temperature Range of 100-340 K

Overview of attention for article published in Advanced Materials, May 2016



? About this Attention Score

SUMMARY

News

Twitter

Title A Centrosymmetric Hexagonal Magnet with Superstable Biskyrmion Magnetic Nanodomains in a Wide Temperature Range of 100-340 K

Published in Advanced Materials, May 2016

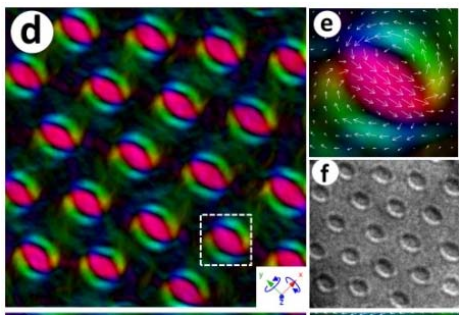
DOI 10.1002/adma.201600889 [↗](#)

国际替代计量 (Altmetrics) 机构对全球531万篇学术文章进行跟踪，结果表明：本论文在发表2个月内，受到的**关注度** (Attention Score) 已经位于所有跟踪文章的 **Top 25%**。

Altmetric has tracked 5,310,968 research outputs across all sources so far. Compared to these this one has done well and is in the 88th percentile: it's in the top 25% of all research outputs ever tracked by Altmetric.

小结

- 共价键-磁性双调控，压制结构相变，建立螺旋磁结构
- 首次在非手性材料中观察到双自旋拓扑态斯格明子
- 室温附近的宽温区，推动磁斯格明子的实际应用



事实再一次证明，传统材料里面确有新东西

W.H.Wang and G.H.Wu et al. *Advanced Materials* 28, 6887 (2016)

总结与展望

- 基于**MMX**合金的特点，以居里温度窗口作为调控磁相变的新思路，实现相稳定性和磁结构的同步调节，获得具有优异磁响应性能的新型磁相变材料。
- 磁性、化学键和能带的协同作用和调控，成功压制结构相变，获得跨室温、宽温域的双斯格明子材料。
- 磁性形状记忆合金、固态磁制冷、热磁发电、磁信息存储等方面具有潜在的应用。

谢谢!





F. Heusler

磁性影响结构的研究方法

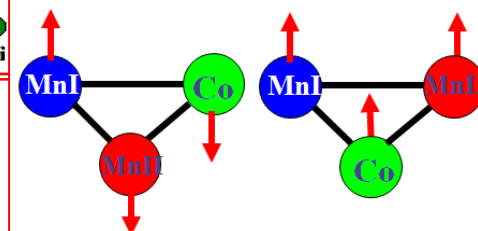
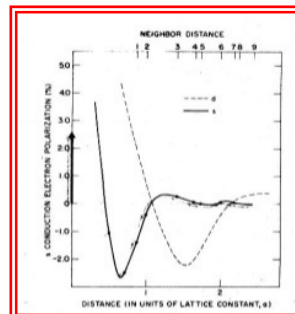
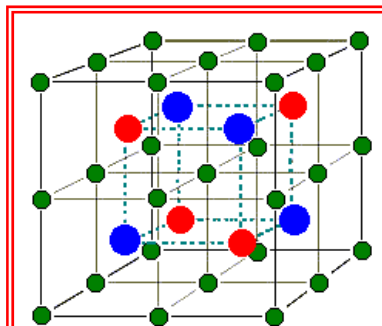
占位规则：价电子多电负性强的占AC位，否则占B位



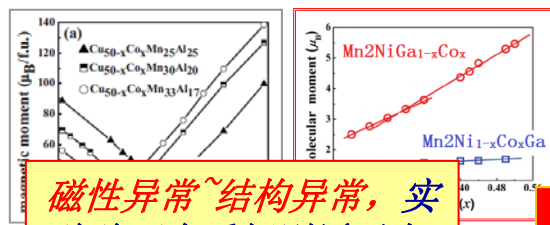
M. Stearns (USA)

Heusler Alloys X_2YZ

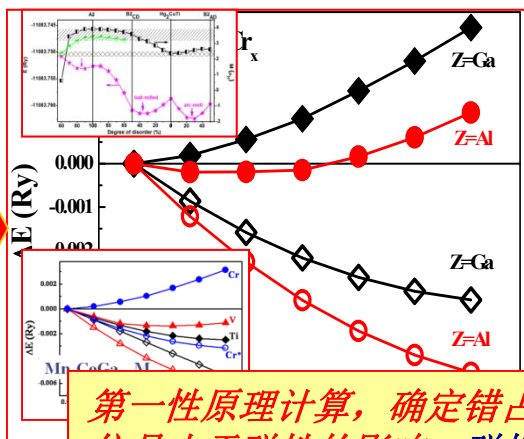
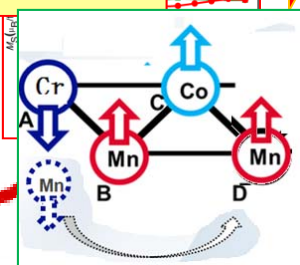
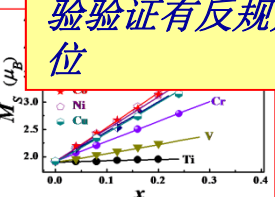
4 Be	Heusler Alloys X_2YZ																5 B	(Z)	
12 Mg																	13 Al	14 Si	
																	31 Ga	32 Ge	33 As
20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As						
38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb						
56 Ba	57-71 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi						
																	81 Tl	82 Pb	83 Bi



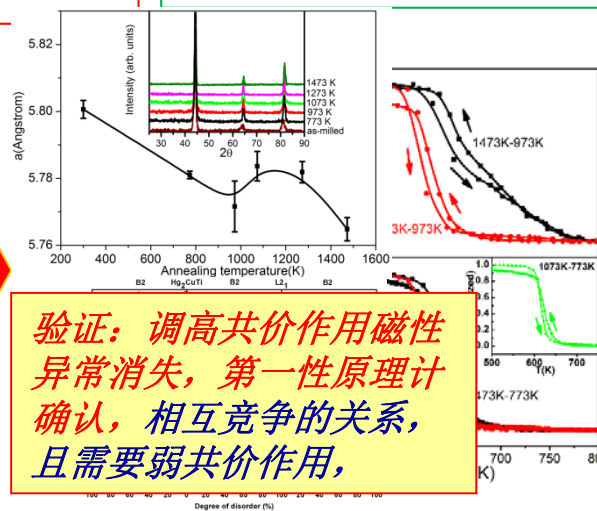
传导电子中的d电子决定磁交换作用。RKKY 自旋极化波



磁性异常~结构异常，实验验证有反规则原子占位



第一性原理计算，确定错占位是由于磁性的影响，磁性可以影响结构



验证：调高共价作用磁性异常消失，第一性原理计算确认，相互竞争的关系，且需要弱共价作用

可以总结一下了

从5类30种材料中总结
“电子合金”观点不适用
要考虑磁性对结构的影响

