

traceDs: An accessible database
of trace element partitioning
experiments

Database goals

Our goal in developing traceDs is to provide a transparent and accessible resource of experimental partitioning data for the community. traceDs now includes all the experimental trace element partitioning data (>5000 experiments).

Database goals

We set a minimum standard for inclusion, with the threshold criteria being the inclusion of:

- Experimental conditions (T,P, capsule, device)
- Major element composition of the phases
- Trace element analyses of the phases

The data are stored using a schema derived from that of the Library of Experimental Phase Relations (LEPR), modified to account for additional metadata, and restructured to permit multiple analytical entries for various element/technique/standard combinations.

What is included in the database?

Experimental determination of partition coefficients

What is NOT included in the database?

- Phenocryst/matrix partition coefficients
- Unpublished data
- Experiments where the compositions are not reported (e.g. just Ds).

Why?

Utility goals

Search methodologies – the current version of the site includes basic search protocols (by phase, conditions, etc.). However, the output is in approximately the same format as the published format. Therefore, care must be taken in processing the data from this raw form into a uniform format. Preprocessed spreadsheets for specific minerals are available through the Earthchem portal

traceDs provides a resource for:

Experimentalists – The database facilitates experimental design, data management plans and data publication.

Reviewers – This resource may be used by reviewers to test models.

Modelers – traceDs may be used to create calibration datasets for trace element partitioning models.

Practitioners – For those who are attempting to calculate differentiation scenarios, the current form allows one to search for compositions that match the system of interest

Characteristics of the experimental partitioning data in traceDs

Similarity with LEPR

experimental apparatus and conditions

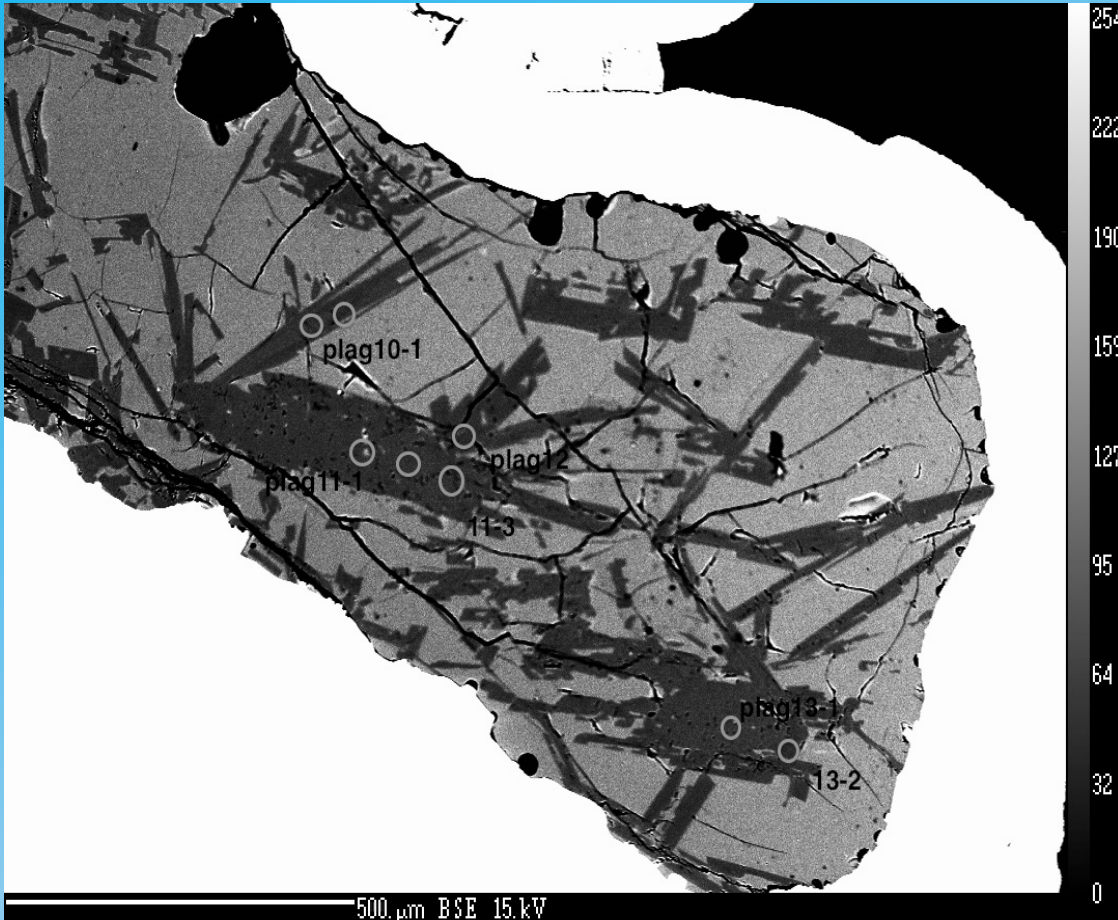
Differences with LEPR

paired phases

multiple analyses of the same element using different analytical techniques

Number of elements analyzed

What is actually represented in the database



Each point represents a spot where a chemical analysis was performed

Typically, analyses of each phase are averaged and reported as pairs

Characteristics of the experimental partitioning data in traceDs

Reference

Temperature(s)

Apparatus

Analytical Procedure

Run time

Pressure

Location of Lab

trace elements

mode

Starting composition

Major elements (all phases)

analytical error

temperature trajectory

Restricted vocabulary

Process of database population

The database was populated paper by paper

Development of the upload template – you have been sent a copy

First recommendation – everyone should publish experimental data using a similar format that can be uploaded

We will revisit the template after the break

What did we learn during the process of population?

Distribution of data in compositional space – Even though we have conducted thousands of experiments – the coverage in compositional space is uneven – result is that we have a great deal of data for some elements/rock types/pressures and none for others.

Over-processed data - We have rarely published the entire analytical dataset – rather, we have analysed the experimental charges, then averaged the results prior to interpretation and publication

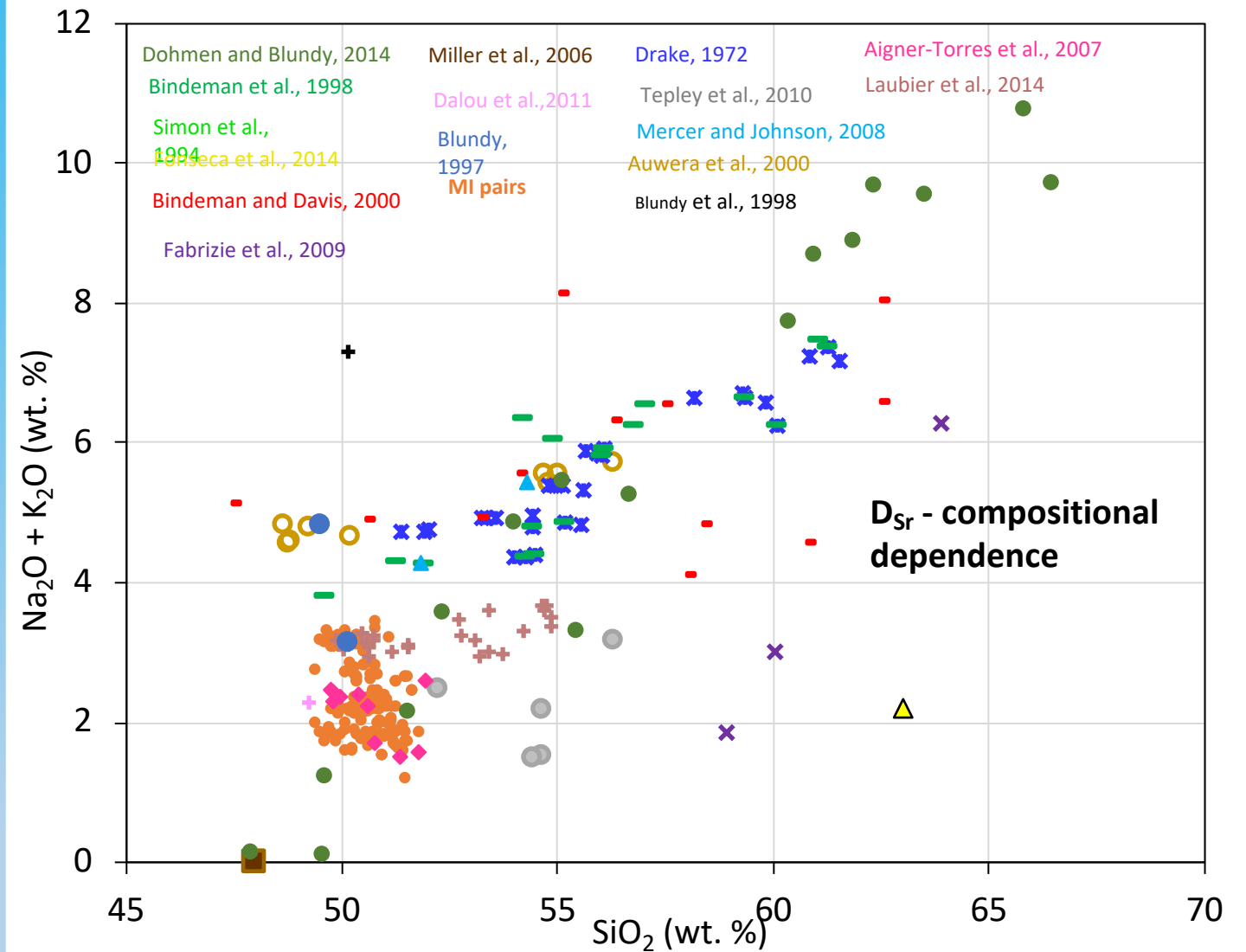
Relevant Citation: Nielsen, R. L., M. Ghiorso, and T. Trishmann (2015), traceDs: What we have learned about the existing trace element partitioning data during the population phase, Abstract V33C-3119 presented at 2015 Fall Meeting, AGU, San Francisco, Calif.

Distribution of data in compositional space – examples from plagioclase/melt experimental data

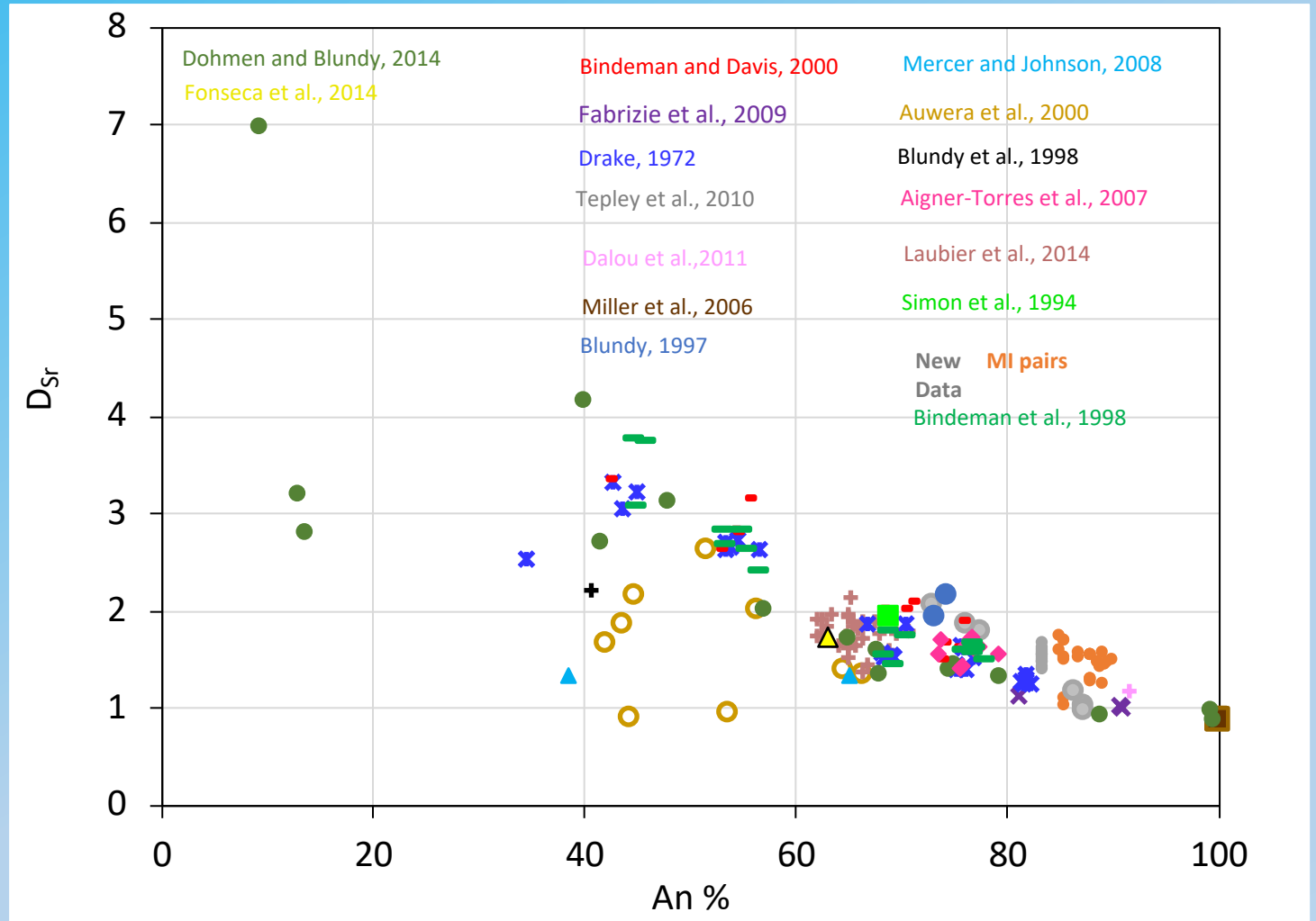
Existing Experimental data for plagioclase/melt partitioning			
Total # of experiments			276
# experiments that have data for each of these elements	Sr		167
	Ba		147
	La		79
	Ce		96
	Lu		25
	Ti		95
	Li		49
	Zr		41
	Pb		41
	Hf		10
	Re		1
	Os		0

Relevant Citation: Nielsen, R.L., Ustunisik, G., Weinsteiger, A.B., Tepley, F.J., Johnston, A.D. and Kent, A J.R., 2017, Trace Element Partitioning Between Plagioclase and Melt: An Investigation of the Impact of Experimental and Analytical Procedures, Geochem Geophys Geosys., DOI 10.1002/2017GC007080

Distribution of data in compositional space – examples from plagioclase/melt experimental data for Sr



Distribution of data in compositional space – examples from plagioclase/melt experimental data for Sr



What can we use this type of information for?

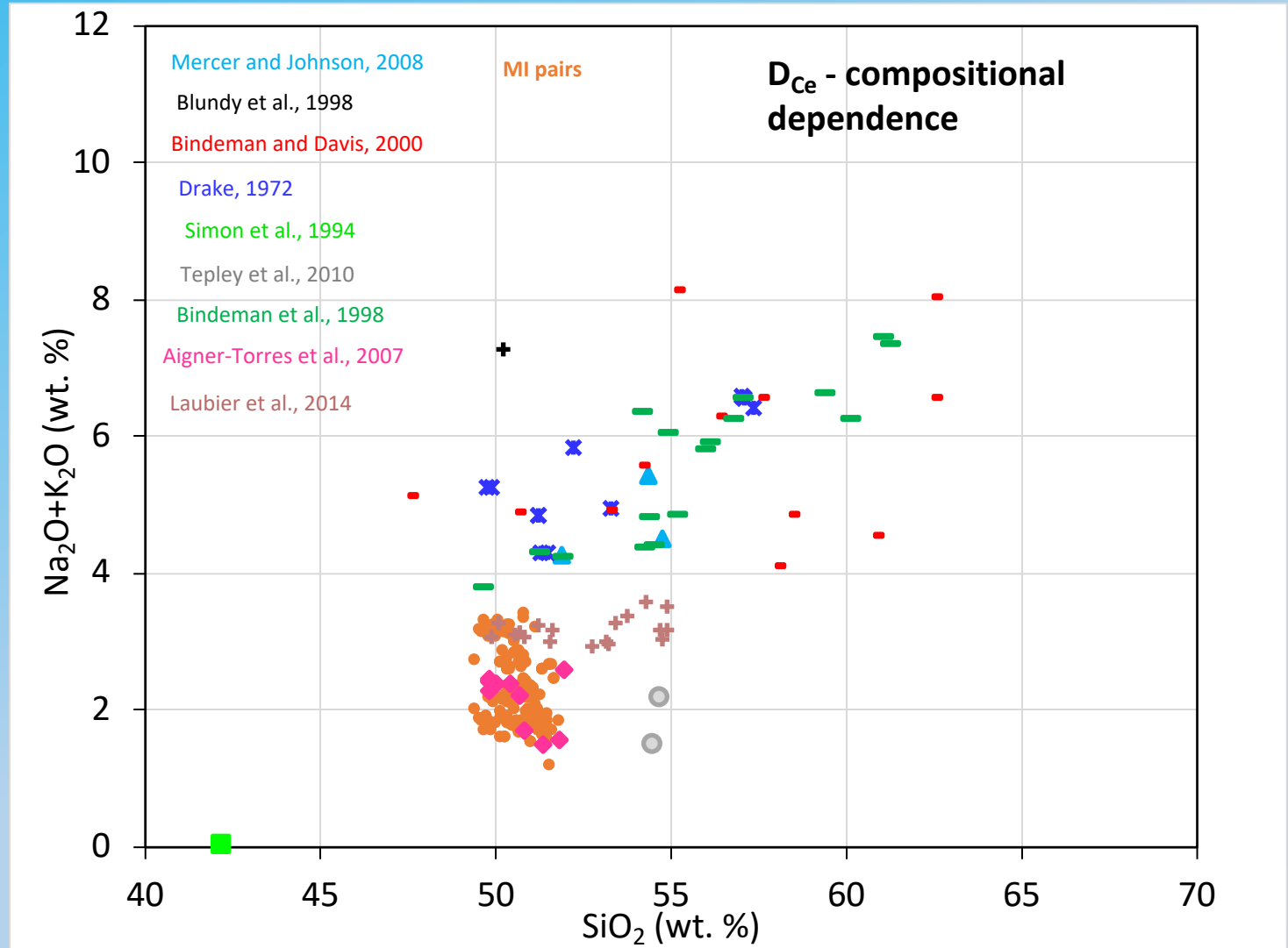
Experimentalists – describe the scope of the existing database.
Describe where the “holes” are.

Modelers – build a calibration dataset (we will do this in the second half of afternoon)

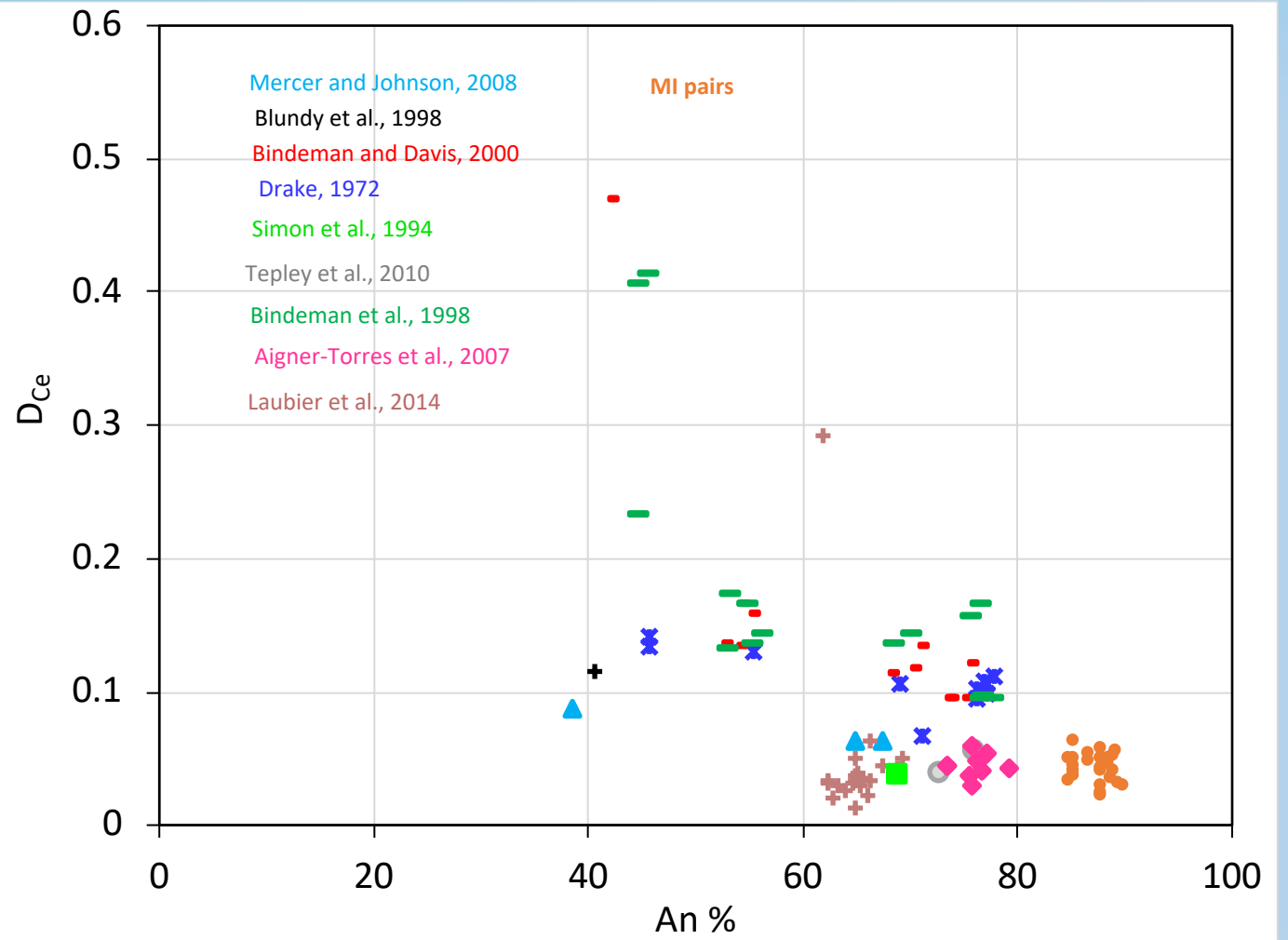
Reviewers – test models that are being submitted for publication

Provides a “ready made” database – previously every investigator had to compile their own

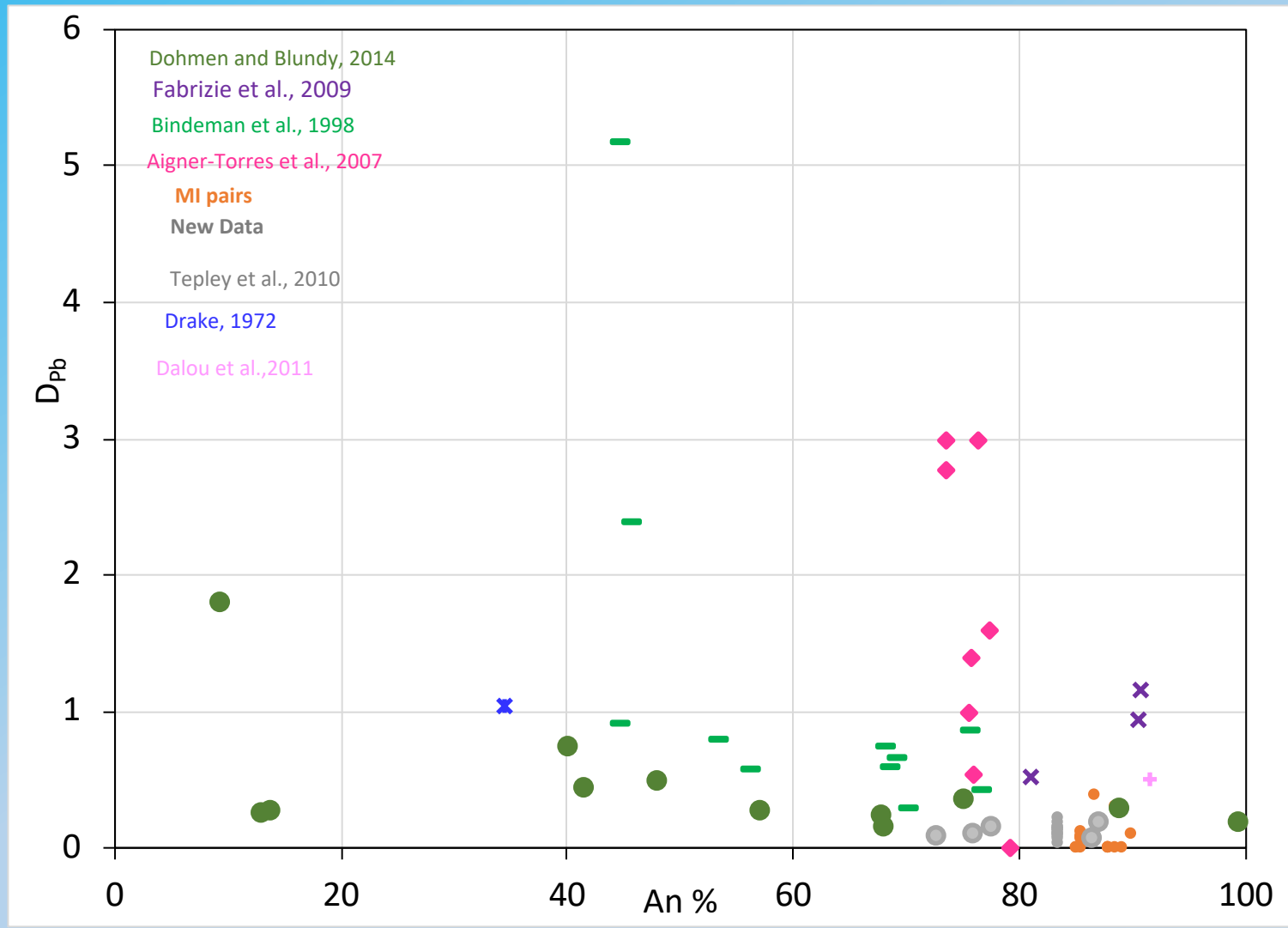
Distribution of data in compositional space – examples from plagioclase/melt experimental data for Ce



Distribution of data in compositional space – examples from plagioclase/melt experimental data for Ce



Distribution of data in compositional space – examples from plagioclase/melt experimental data for Pb



So – why so much scatter

Temperature, pressure and compositional dependence – we can build models based on those parameters – and will make some efforts towards that in the second part of the afternoon

Analytical and experimental error – which has a greater impact as the partition coefficient drops – let's see why and what the impact can be

Now what do I do?

To understand how to model trace element partitioning you need to understand the character of the compositional, T and P dependencies – that requires that we first understand the sources of error and its impact

**Let us look at how experimental data is processed
and how you can avoid making systematic errors
when using published data**

Sources of experimental and analytical error

- **Contamination – more than a single phase represented in an analysis**
- **Relic heterogeneity from dopant addition**
- **Loss of component to capsule or volatilization**

Sources of processing error

- Documentation error in laboratory
- Publication error – editorial/typo
- Transcription error
- Upload and download error
- Processing error – mistakes made while using the information.

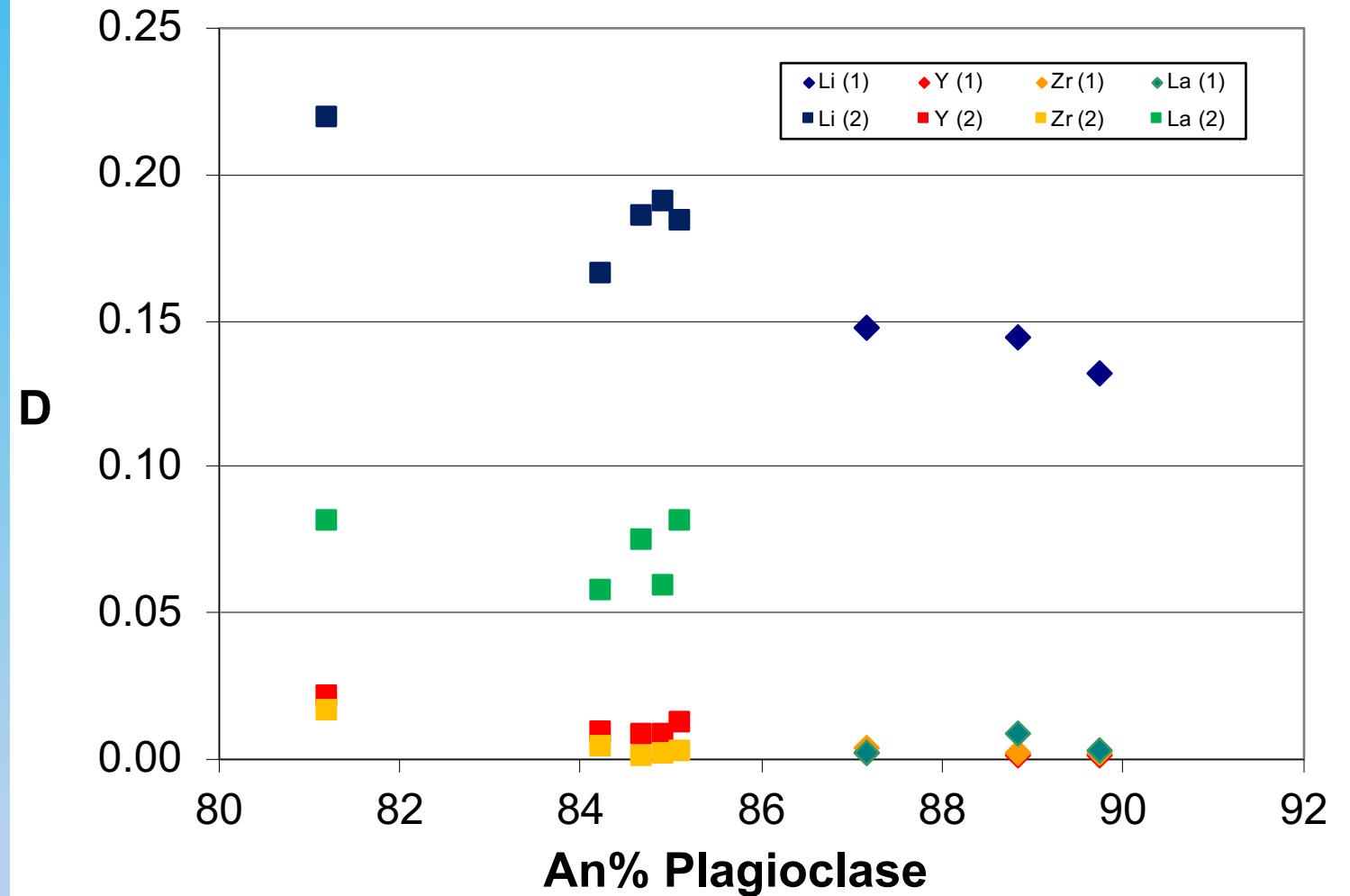
The creation of any database is a human endeavour –

Our goal is to work to improve the collective database and avoid re-inventing the wheel

Most important, if you see something that you think is an error – tell me so that we can fix it.

**Low pressure experiments
on the partitioning of select
elements between
plagioclase and basaltic
liquid (Nielsen et al. MS in
prep)**

**Two sets of experiments
Set 1 – 1230 C for 24 hours
Set 2 – 1300 C for 1 hour
then dropped to 1230 C for
24 hours**



Resultant low Ds and variations are related to relic cores and in addition are a consequence of the dopant acting as a flux – not necessarily a Henry's Law issue

In developing new experimental procedures, we need to balance the need to add dopants for highly incompatible elements in order to enhance analytical precision and the need to keep the composition as close as possible to natural levels

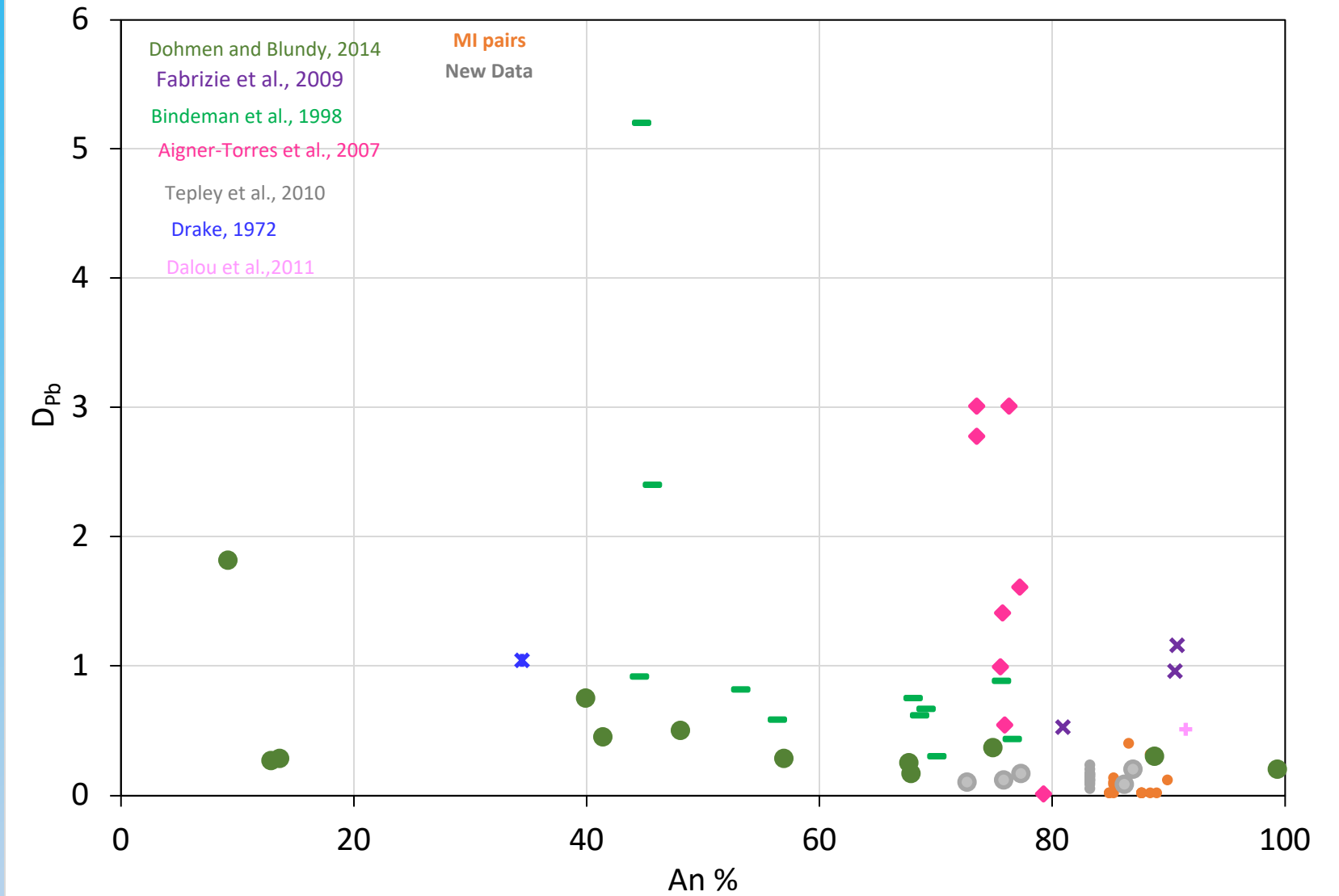
In examining the database, you can make the decision to use either doped or undoped experiments, simple/complex temperature trajectory, etc. – so long as there is sufficient data to do so

Pb partitioning between plagioclase and melt

What is going on?

Dopant volatilization after initial crystallization

Result – anomalously high D



Plagioclase-melt partitioning experiment

What do we see when we look at the data in detail?

Experiment TE-32

Starting composition Gorda Ridge

MORB D9-1

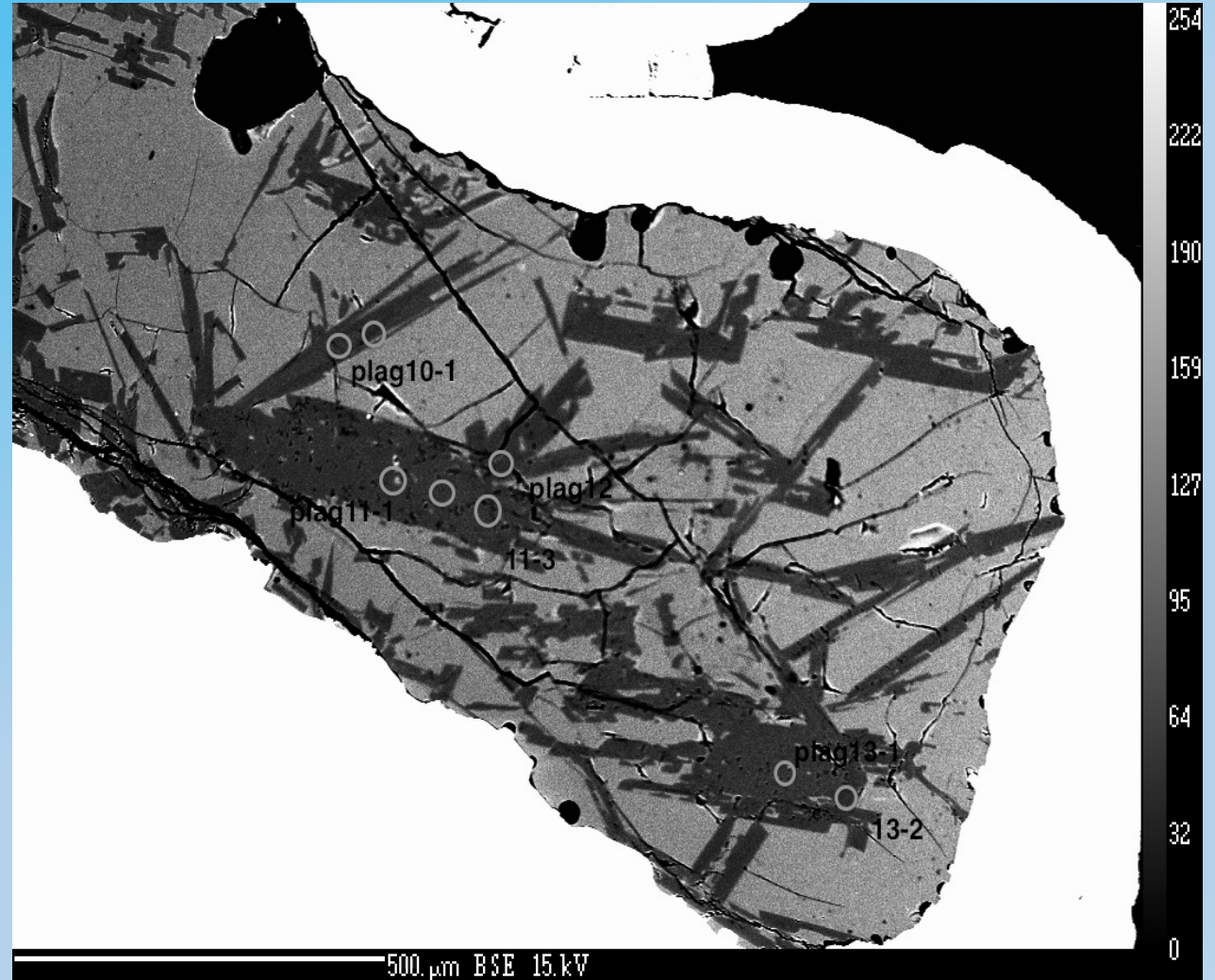
Doped with ~100 PPM

of several trace elements

1% wt % H₂O added

1300 °C initial heating for 1 hour

5 kb, 1210 °C for 24 hours



Ce partitioning between plagioclase and melt

What is going on?

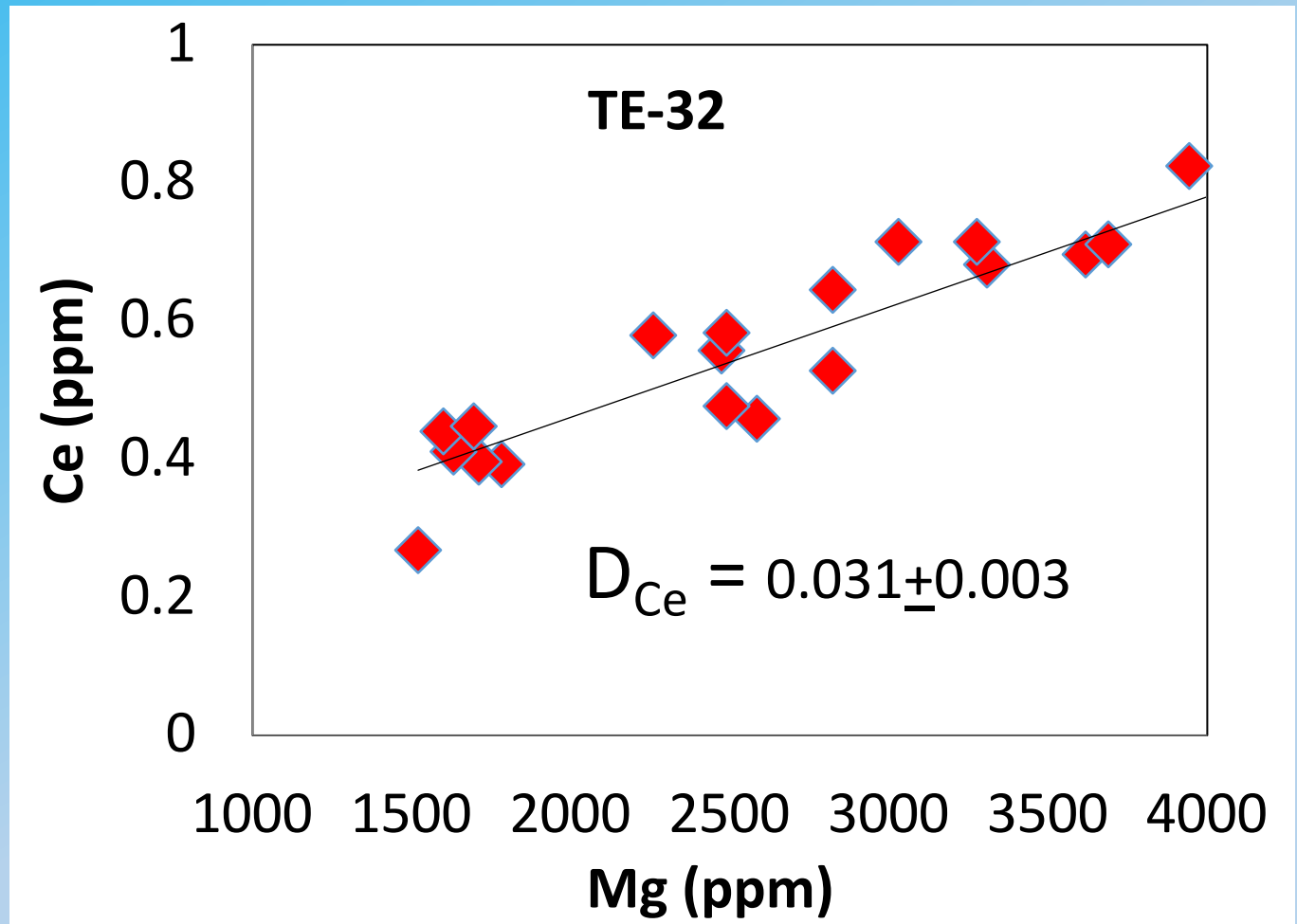
Each spot is a single analysis by laser ICP-MS

Intent was to analyze plagioclase and co-existing glass

Plot to right is the low Mg data (presumed to be plagioclase)

What do we average?

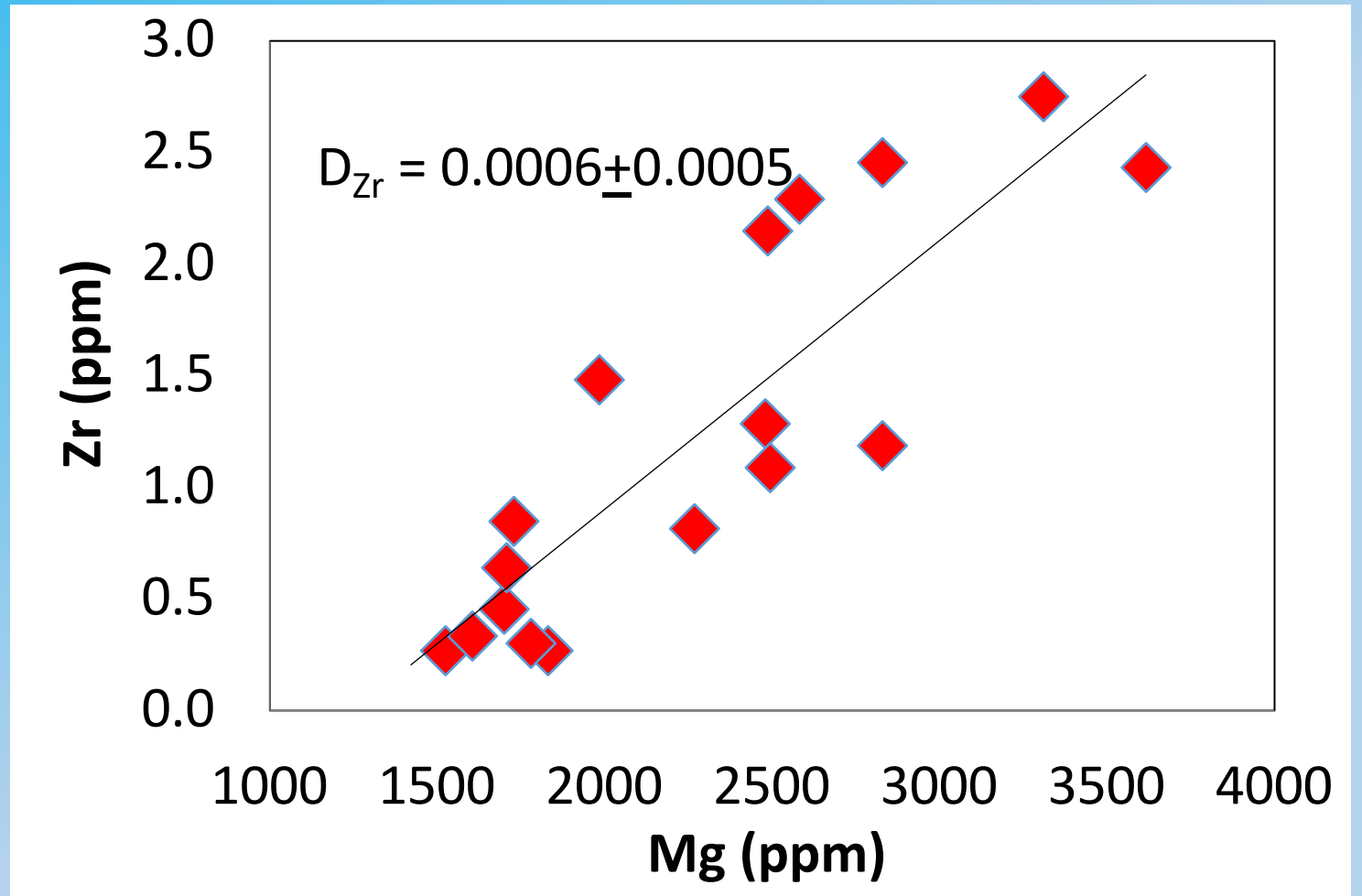
Result – anomalously high D



Zr partitioning between plagioclase and melt

Effect of contamination increases as D decreases

Result – anomalously high D



Impact of “mixed” analyses on calculated Ds

As D drops – the proportional impact of a small addition of another phase increases

Why is this important?

It introduces a systematic bias to measurements of partition coefficients that get included in numerical expressions

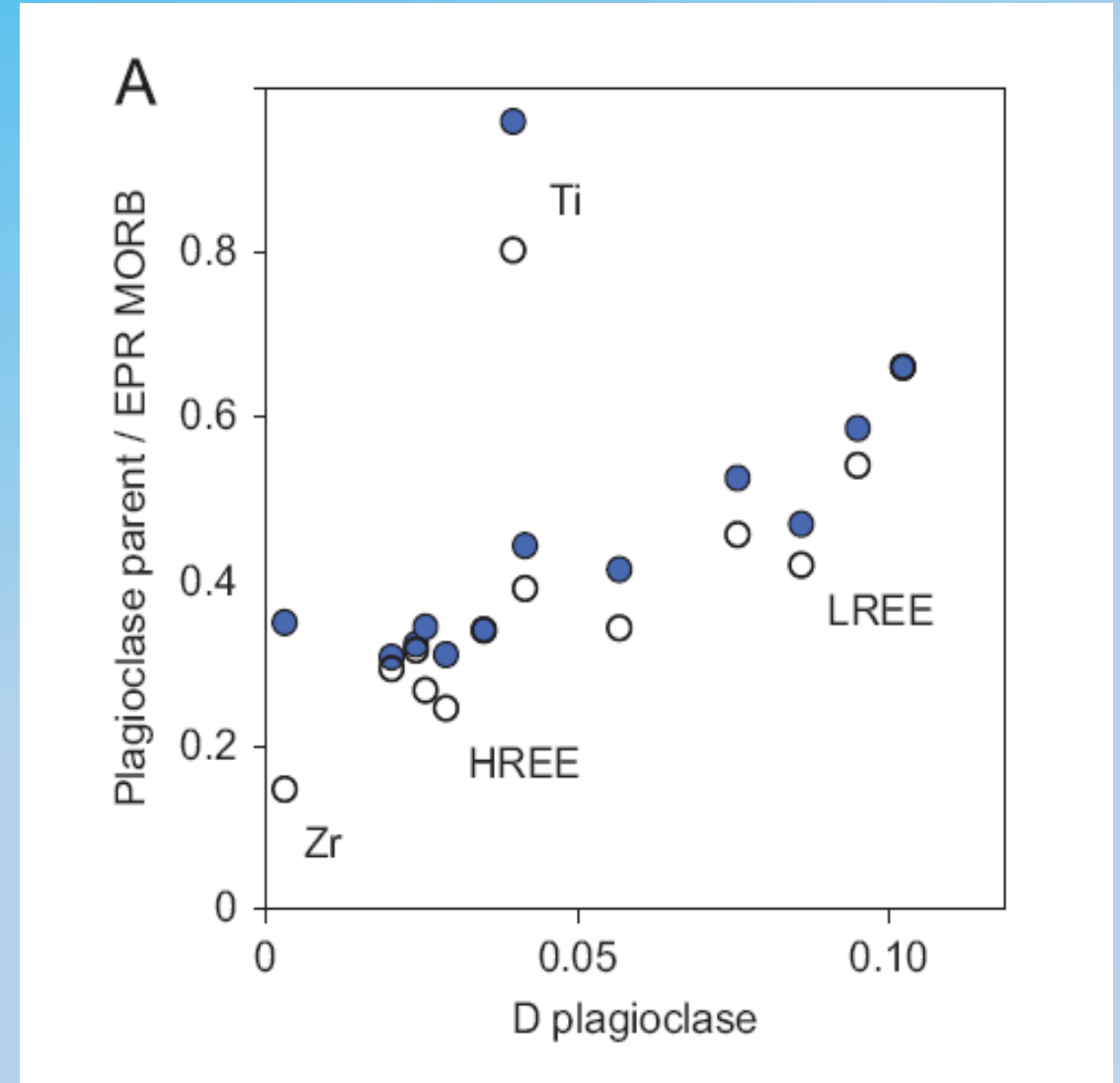
We will discuss this as we process data in groups later

D^{true}	99% plagioclase 1% glass (D^{mix})	$D^{\text{mix}}/D^{\text{true}}$
1	1	1.00
0.5	0.505	1.01
0.1	0.109	1.09
0.05	0.0595	1.19
0.01	0.02	2.0
0.005	0.015	3.0
0.001	0.011	11.0

Table 4. Influence of analytical error related to the inclusion of glass in analyses of plagioclase on the values of the estimates of plagioclase/melt partition coefficients. The “true” D value (D^{true}) assumes that analyses of plagioclase in the mineral/glass pair is pure. D^{mix} is the estimated value of D assuming that the analytical volume includes 99 % plagioclase and 1% glass.

Impact of “mixed” analyses on calculated Ds

from Lissenberg et al., 2013 “the degree of trace element depletion of plagioclase relative to MORB correlates strongly with plagioclase D’s, which would require the D’s to be increasingly erroneous with increasing incompatibility —an unlikely coincidence”



Impact of “mixed” analyses on calculated Ds

As D drops – the proportional impact of a small addition of another phase increases

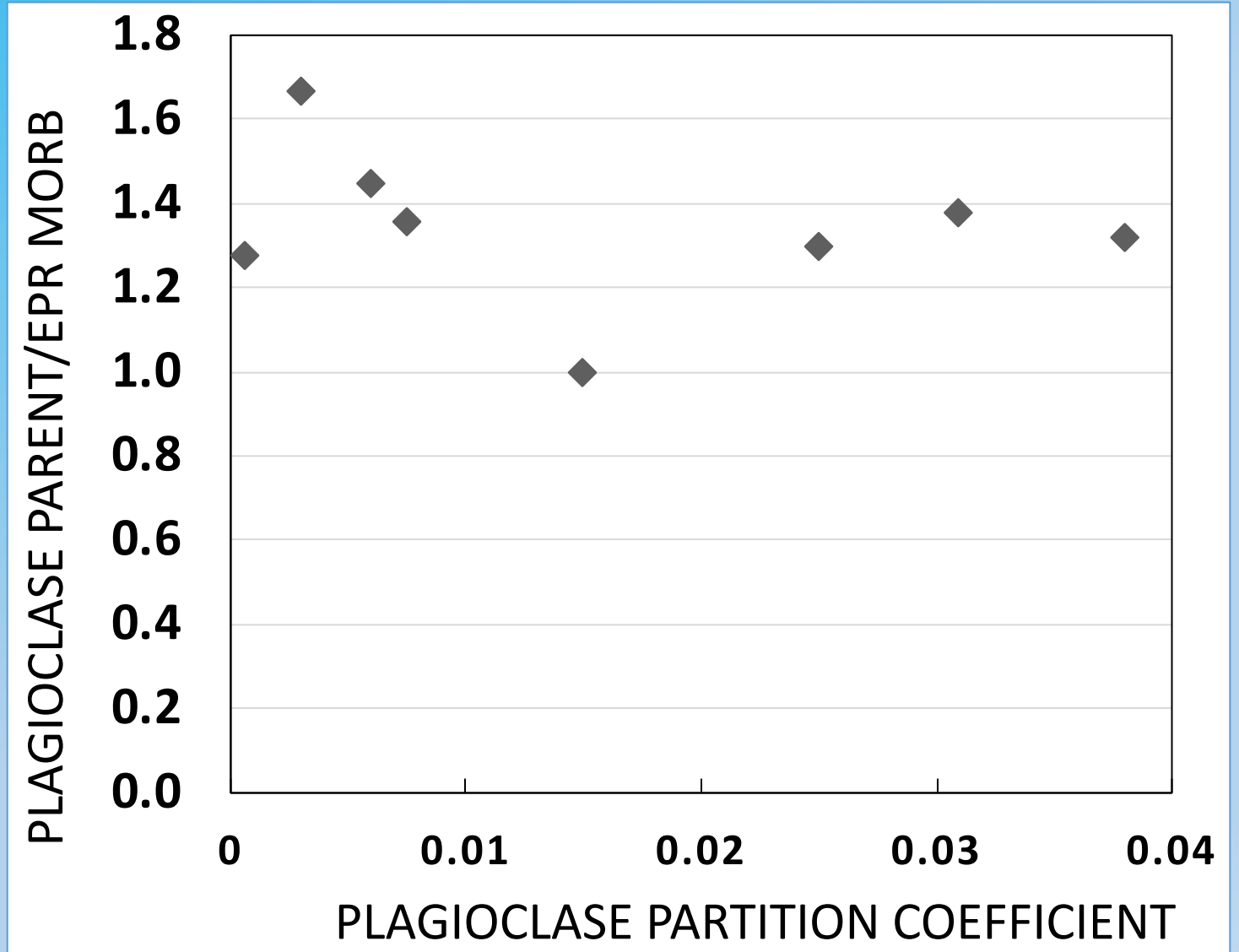
Why is this important?

We can examine the impact of this systematic bias by re-interpreting the Lissenberg data using another set of partition coefficients developed for a specific composition – in this case based on experiments on MORB.

	D plag Nielsen	D plag Bedard	Ratio
Ti	0.025	0.04	1.6
La	0.038	0.09	2.4
Ce	0.031	0.075	2.4
Sm	0.015	0.06	4.0
Gd	0.0075	0.03	4.0
Y	0.006	0.03	5.0
Lu	0.003	0.02	6.7
Zr	0.0006	0.005	8.3

If we use the alternate partition coefficients to interpret the same data, we find that the model results are fundamentally different – in fact they suggest the opposite conclusion – e.g. within error the plagioclase phenocrysts are in equilibrium with their host.

Take away message – be careful that you understand the underlying dependencies when you calculate a numerical expression



**OK – now that we have all these
cautionary tales – how can we use the
database to solve problems?**

Example from Spinel/melt partitioning experiments

Search for compositional dependencies

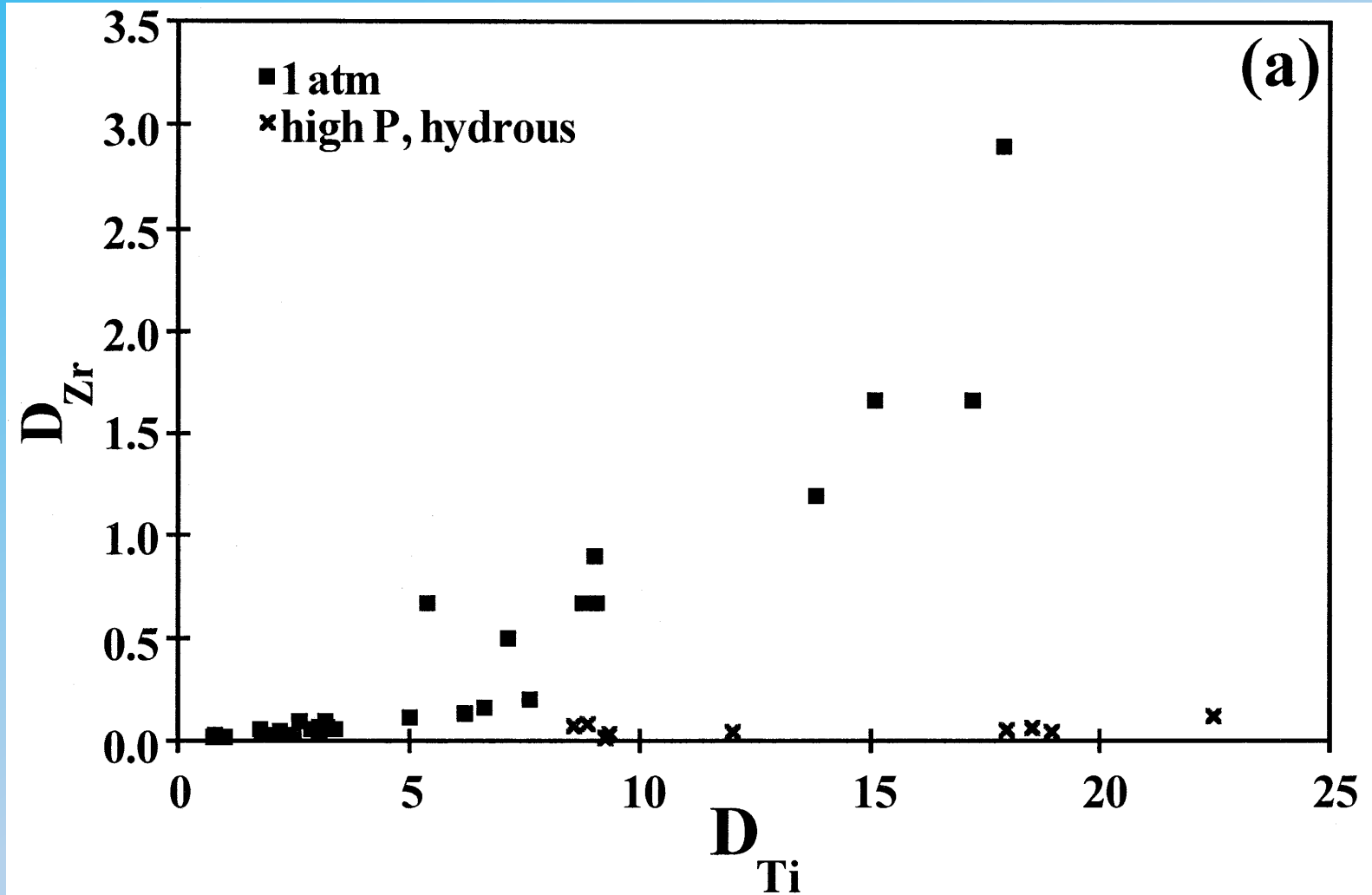
Relevant Citation: Nielsen, RL and Beard, JS, 2000, Magnetite-melt HFSE partitioning, Chem. Geology, 164, 21-34
[https://doi.org/10.1016/S0009-2541\(99\)00139-4](https://doi.org/10.1016/S0009-2541(99)00139-4)

Example from Spinel/melt
partitioning experiments
Search for compositional
dependencies

Experimental data on spinel/melt
partitioning Nielsen and Beard,
2000

Include chromite and magnetite
Both 1 atm and high pressure data

To be able to predict partitioning
behaviour, you need to understand
the controlling parameters

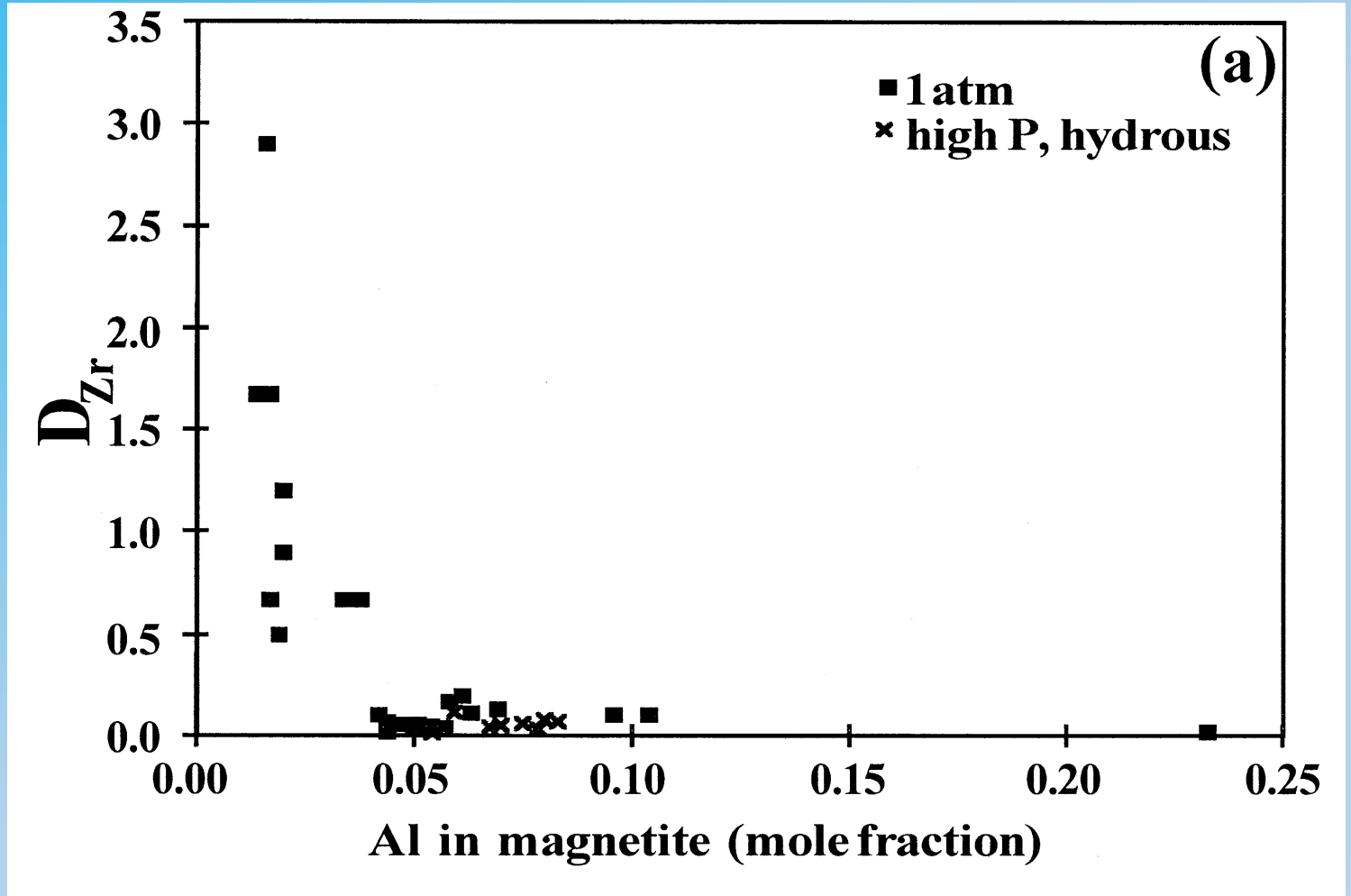


Example from Spinel/melt
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Search for compositional
dependencies

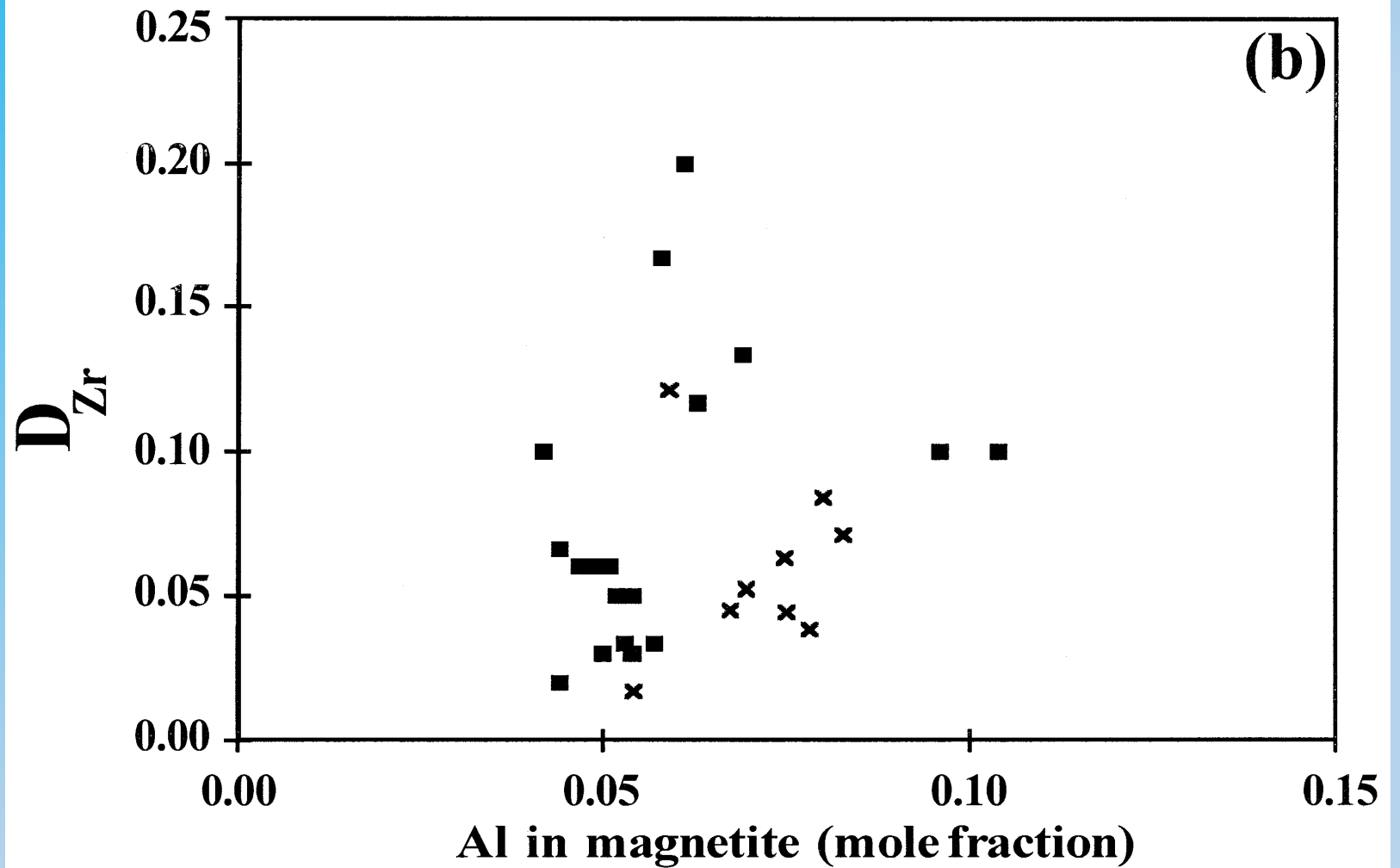
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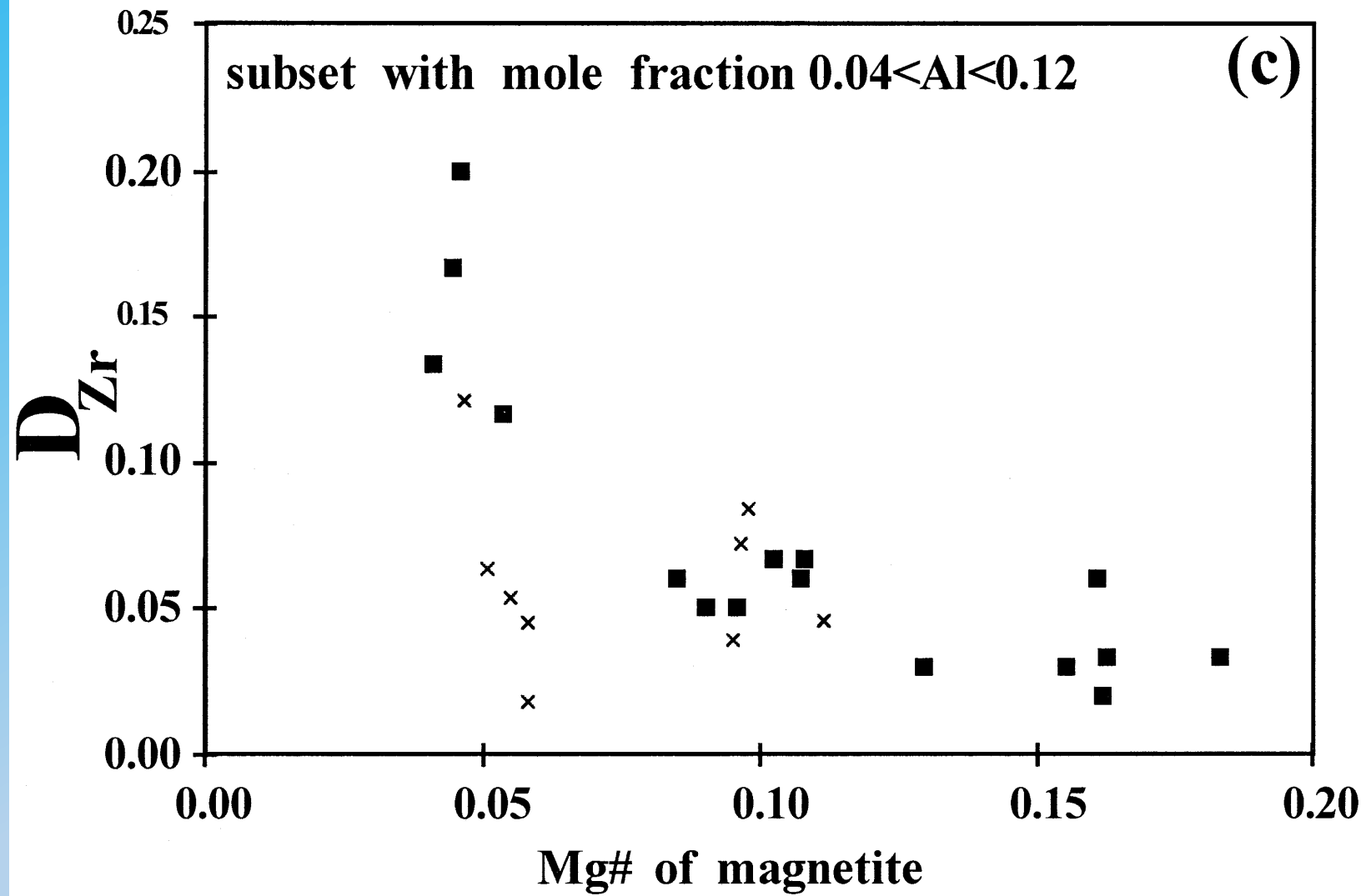
To be able to predict partitioning
behaviour, you need to understand
the controlling parameters



We can examine a dataset by considering a subset of the information. In this case, we are looking at a small section of the database (~4 -12 mole fraction). We can look at other controlling parameters by “rotating” the data



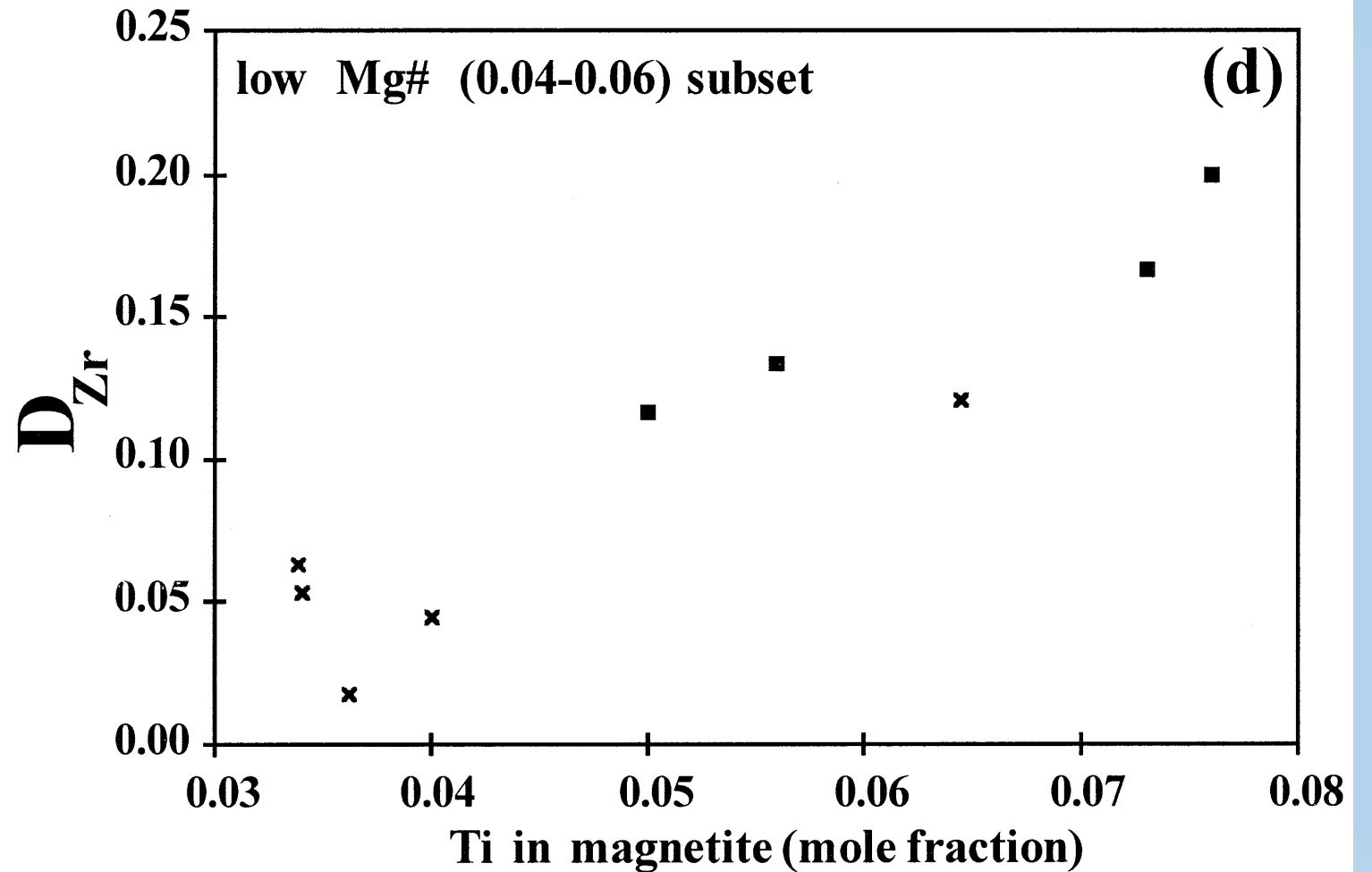
Restricting ourselves to a subset of the data, we can see some dependence on Mg# of the spinel



Further subdividing the data to a narrow range of Mg # yields a linear trend for the data

This is attributed to the impact of non ideal mixing of spinel components – particularly the HFSE components

Taking all the dependencies together allows us to calculate a numerical expression that describes spinel/melt partitioning



An alternate approach is to use an elastic strain model – however that approach is less useful when there are complex mixing properties for the trace element components.

Such an approach requires a large experimental dataset. In the past 16 years new data has been published and included in the traceDs database – and the old expression has not been re-tested or re-calibrated

$$\begin{aligned} \ln D_{\text{HFSE}} = & C_0 + C_1 \ln D_{\text{Ti}} + C_2(\text{Ti in magnetite}) \\ & + C_3(\text{Al in magnetite}) \\ & + C_4(\text{Mg exchange}) \\ & + C_5(\text{Ti/Al in magnetite}) \\ & + C_6 P(\text{kbar}) + C_7(10\,000/T(\text{K})) \end{aligned}$$