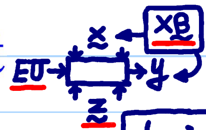
Epitaxial Layer Growth Experiment

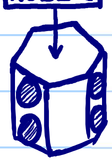


previous exp'ts & designs in CH3 (comparative exp'ts) $Y = X\beta + \varepsilon$

factorial design (因子設計) ← multi-way layout
→ often used in exp'ts with a larger # of factors ← cf. →

- An AT&T experiment based on 2^4 design; in industrial era four treatment factors each at two levels. ★response: thickness
  There are 6 replicates for each of the 16 ($=2^4$) level combinations; data given on LNp.5-2.

nozzle



treatments

★treatment factors: A, B, C, D

Q: Why is fewer # of levels often used in factorial exp'ts? → All 2 levels — $-1, +1$

"Qualitative or quantitative" is not an important issue in 2-level case [why? both can use (0,1) or (−1,1) codings]

qualitative or quantitative?

Table 1: Factors and Levels, Adapted Epitaxial Layer Growth Experiment

Treatment Factor	Level −	Level +
A. susceptor-rotation method	continuous	oscillating
B. nozzle position	2	6
C. deposition temperature (°C)	1210	1220
D. deposition time	low	high

★Exp'tal unit: a group of 6 wafers

homogeneous — EU$_1$ • • • EU$_{16}$

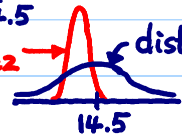
r (A, B, C, D) r

⇒ 16 whole plots, 96 subplots

⇒ all 4 factors are WP factors

cf. → the objectives in the comparative exp'ts

◉ **Objective** : Reduce variation of y (=layer thickness) around its target 14.5 μm by changing factor level combinations.



Data from Epitaxial Layer Growth Experiment

$E(y_A) = \beta_0 + \beta_1 x_A$

All d.f. = 10 = 2 + 8

for parameters β ↑ ↑ for $Var(y) = \sigma^2$

2^4 full factorial design

Table 2: Design Matrix and Thickness Data, Adapted Epitaxial Layer Growth Experiment

unreplicated

★conceptual model:
$y \sim \beta_0 + A + B + C + D + AB + AC + AD + BC + BD + CD + ABC + ABD + ACD + BCD + ABCD + \varepsilon$ (sum coding)

for Thickness | for $\bar{y}$/ s^2/ $\ln(s^2)$

Run	A	AB	B	C	D	Thickness						$\bar{y}$	s^2	$\ln s^2$
1	−	+	−	−	+	14.506	14.153	14.134	14.339	14.953	15.455	14.59	0.270	−1.309
2	−	+	−	−	−	12.886	12.963	13.669	13.869	14.145	14.007	13.59	0.291	−1.234
3	−	+	−	+	+	13.926	14.052	14.392	14.428	13.568	15.074	14.24	0.268	−1.317
4	−	+	−	+	−	13.758	13.992	14.808	13.554	14.283	13.904	14.05	0.197	−1.625
5	−	−	+	−	+	14.629	13.940	14.466	14.538	15.281	15.046	14.65	0.221	−1.510
6	−	−	+	−	−	14.059	13.989	13.666	14.706	13.863	13.357	13.94	0.205	−1.585
7	−	−	+	+	+	13.800	13.896	14.887	14.902	14.461	14.454	14.40	0.222	−1.505
8	−	−	+	+	−	13.707	13.623	14.210	14.042	14.881	14.378	14.14	0.215	−1.537
9	+	−	−	−	+	15.050	14.361	13.916	14.431	14.968	15.294	14.67	0.269	−1.313
10	+	−	−	−	−	14.249	13.900	13.065	13.143	13.708	14.255	13.72	0.272	−1.302
11	+	−	−	+	+	13.327	13.457	14.368	14.405	13.932	13.552	13.84	0.220	−1.514
12	+	−	−	+	−	13.605	13.190	13.695	14.259	14.428	14.223	13.90	0.229	−1.474
13	+	+	+	−	+	14.274	13.904	14.317	14.754	15.188	14.923	14.56	0.227	−1.483
14	+	+	+	−	−	13.775	14.586	14.379	13.775	13.382	13.382	13.88	0.253	−1.374
15	+	+	+	+	+	13.723	13.914	14.913	14.808	14.469	13.973	14.30	0.250	−1.386
16	+	+	+	+	−	14.031	14.467	14.675	14.252	13.658	13.578	14.11	0.192	−1.650

AC, ⋯ ABC, ⋯ ABCD

Thickness ← replicated

check LNp.4-65

The # of different level combinations in the exp't ⇒ can be used to study 16 parameters (1 intercept, 15 effects)

model matrix

contain what information?

$E(y_x)$ and $Var(y_x)$ ← pure error information

assume equal variance? or unequal variance?

① response: Thickness
# of all obs. = 16×6 = 96
all d.f.
16 → for effects
80 → for Var(ε)

② response: $\bar{y}$/ s^2/ $\ln s^2$
# of all obs. = 16
all d.f.
16 → for effects
0 → for Var(ε)

❖ **Reading**: textbook, 4.1

2^k Designs: A General discussion

of distinct level combinations

# of levels

# of factors

- Full factorial design (全因子設計)
- $2 \times 2 \times \ldots \times 2 = 2^k$ design.

Actually, 2^k full factorial design
⇒ an OA of strength k
(orthogonality of design matrix)
⇒ All effects in model matrix are geometrically orthogonal (under sum codings)

cf. Design matrix → + model + codings

- Planning matrix vs model matrix → $Z = XB + E$
  (see Tables 4.3, 4.5, textbook, p.158 & 161).

← randomization

- Run order and restricted randomization
  (see Table 4.4, textbook, p.160).

∵ factor C is a hard-to-change factor
⇒ each of its 2 levels 1210, 1220°C only performs once

C: + & −
whole
sub
EU1 ··· EU8 EU9 ··· EU16
(A, B, D) (A, B, D)

Q: When can we ignore the split-plot structure? Ans. whole-plot errors have small variance.

- *Balance*: each factor level appears the same number of times in the design matrix.
- *Orthogonality* : for any pair of factors, each possible level combination appears the same number of times in the design matrix.

defined on DM

OA of strength 1
⇒ In model matrix, ME ⊥ $\mathbb{1}$.

OA of strength 2 sum codings
⇒ In model matrix, ME ⊥ ME

- Replicated vs unreplicated experiment.
  Thickness $\bar{y}/s^2/\ln s^2$

Replicates can bring in information about $Var(Z_X) \longleftrightarrow X$

❖ **Reading**: textbook, 4.2

Main effects and Plots

can be referred to as a parameter, or an estimator

- Main effect of factor A:

parameter → $ME(A) = \bar{\mu}(A+) - \bar{\mu}(A-)$,

estimator → $ME(A) = \bar{\bar{z}}(A+) - \bar{\bar{z}}(A-)$.

∵ orthogonality.

check LNp.2

The averages are taken over all level combinations of (B, C, D)

consider the collection as a population of (B, C, D) and apply random effect model for (B, C, D)

- Advantages of factorial designs (R.A. Fisher): *reproducibility* and *wider inductive basis* for inference.

cf. OFAT (LNp.13), effect of A defined as:
$\bar{\mu}(A+ \mid (B,C,D) = x^*) - \bar{\mu}(A- \mid (B,C,D) = x^*)$

- Informal analysis using the **main effects plot** can be powerful.

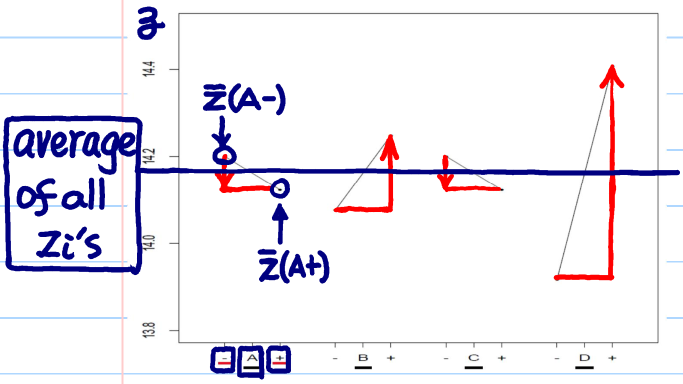


Figure 1: Main Effects Plot, Adapted Epitaxial Layer Growth Experiment

response. In the case, z can be Thickness / $\bar{y}$ / s^2 / $\ln s^2$

Let $\mu_{ABCD} = E(z_{ABCD})$
a level combination

e.g. $\mu_{++++} = E(z_{++++})$
⋮
$\mu_{+--+} = E(z_{+--+})$
⋮

Interaction Effects

$\bar{z} \longrightarrow \bar{\mu}$
estimator parameter

cf. $ME(B) = \bar{z}(B+) - \bar{z}(B-)$

- **Conditional main effect** of B at $+$ level of A (or $-$ level of A):

check LNp.2

$$ME(B|A+) = \overbrace{\bar{z}(B+|A+)}^{=\bar{z}(A+B+)} - \overbrace{\bar{z}(B-|A+)}^{=\bar{z}(A+B-)}.$$

$$ME(B|A-) = \underbrace{\bar{z}(B+|A-)}_{=\bar{z}(A-B+)} - \underbrace{\bar{z}(B-|A-)}_{=\bar{z}(A-B-)}.$$

significant INT(A,B)
⇒ the effect magnitude of B changes with the setting of A

- **Two-factor interaction effect** between A and B:

$$INT(A,B) = \frac{1}{2}\{ME(B|A+) - ME(B|A-)\}$$

becomes large when the lines in the interaction plot are not parallel.

$$= \frac{1}{2}\{ME(A|B+) - ME(A|B-)\}$$

average of 1/4 observations

$$= \underbrace{\frac{1}{2}\{\overbrace{\bar{z}(A+|B+)}^{=\bar{z}(A+B+)} + \overbrace{\bar{z}(A-|B-)}^{=\bar{z}(A-B-)}\}}_{=\bar{z}(A+B+\text{ or }A-B-)} - \underbrace{\frac{1}{2}\{\overbrace{\bar{z}(A+|B-)}^{=\bar{z}(A+B-)} + \overbrace{\bar{z}(A-|B+)}^{=\bar{z}(A-B+)}\}}_{=\bar{z}(A+B-\text{ or }A-B+)}, \quad (1)$$

average of ½ observations

$A \cdot B = +$ $\qquad$ $A \cdot B = -$

- The first two definitions in (1) give more insight on the term "interaction" than the third one in (1). The latter is commonly used in standard texts.

Interaction Effect Plots

Q: What information are contained in the plot? — intercept, 2 main effects, interaction effect

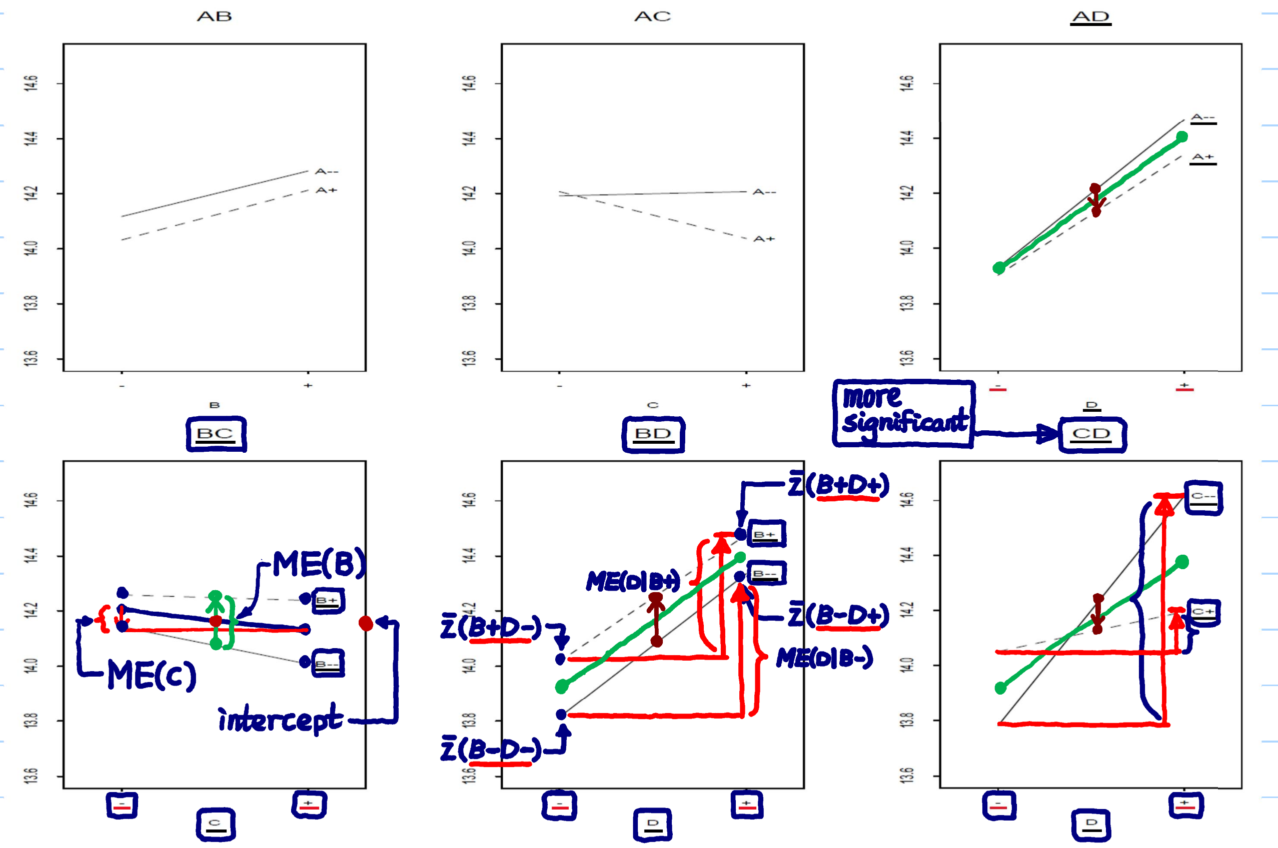


Figure 2: Interaction Plots, Adapted Epitaxial Layer Growth Experiment

Synergistic and Antagonistic Plots

同向作用 反向作用

定性資訊

- An A-against-B plot is *synergystic* if
$$\text{ME}(B|A+) \times \text{ME}(B|A-) > 0,$$
and *antagonistic* if
$$\text{ME}(B|A+) \times \text{ME}(B|A-) < 0.$$

- An antagonistic plot suggests a more *complex* underlying relationship than what the data reveal.

carry same information about ME(C), ME(D), INT(C,D)

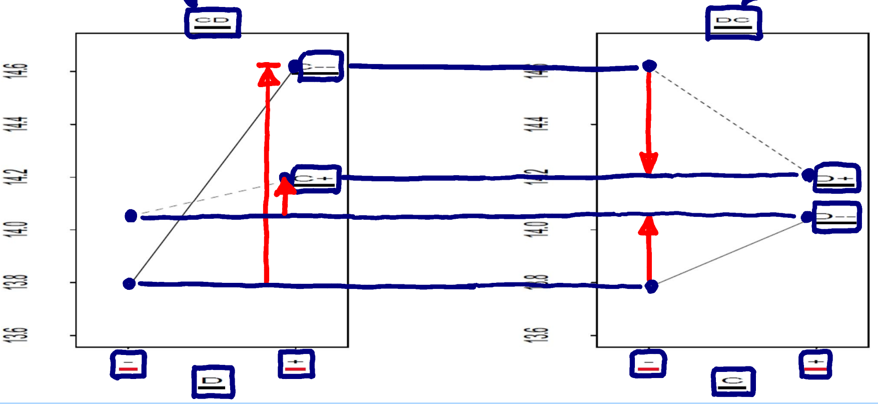


Figure 3: C-against-D and D-against-C Plots, Adapted Epitaxial Layer Growth Experiment

More on Factorial Effects

$= \frac{1}{2}\{[\bar{z}(A+B+C+)+\bar{z}(A-B-C+)] - [\bar{z}(A+B-C+)+\bar{z}(A-B+C+)]\}$

$= \frac{1}{2}\{[\bar{z}(A+B+C-)+\bar{z}(A-B-C-)] - [\bar{z}(A+B-C-)+\bar{z}(A-B+C-)]\}$

$\frac{1}{4}[\text{ME}(A|B+C+)-\text{ME}(A|B-C+)]$

$-\frac{1}{4}[\text{ME}(A|B+C-) - \text{ME}(A|B-C-)]$

3 f.i.

- $\text{INT}(A,B,C) = \frac{1}{2}\text{INT}(A,B|C+) - \frac{1}{2}\text{INT}(A,B|C-)$
$$= \frac{1}{2}\text{INT}(A,C|B+) - \frac{1}{2}\text{INT}(A,C|B-) = \frac{1}{2}\text{INT}(B,C|A+) - \frac{1}{2}\text{INT}(B,C|A-).$$

k f.i.

- $\text{INT}(A_1,A_2,\ldots,A_k)$ (exercise) $= \bar{z}(A\cdot B\cdot C=+) - \bar{z}(A\cdot B\cdot C=-)$
$$= (1/2)\,\text{INT}(A_1,A_2,\ldots,A_{k-1}|A_k+) - (1/2)\,\text{INT}(A_1,A_2,\ldots,A_{k-1}|A_k-).$$
(exercise) $= \bar{z}(A_1\cdot A_2\cdots A_k=+) - \bar{z}(A_1\cdot A_2\cdots A_k=-)$

- A general factorial effect

estimator $\rightarrow \hat{\theta} = \bar{z}_+ - \bar{z}_-$, $\xrightarrow{\text{estimate}}$ $\theta = \bar{\mu}_+ - \bar{\mu}_-$ (parameter)

Note. The definition of the factorial effect parameters is irrelevant to the design matrix.

where $\bar{z}_+$ and $\bar{z}_-$ are averages of one half of the observations. If N is the total number of observations,

$Z = X\beta + \varepsilon$ — all factorial effects (see LNp.2)

$Z \sim N(X\beta, \sigma^2 I)$
$$Var(\hat{\theta}) = \frac{\sigma^2}{N/2} + \frac{\sigma^2}{N/2} = \frac{4}{N}\sigma^2,$$

cf. $\hat{\beta} = (X^T X)^{-1} X^T Z = \frac{1}{N} X^T Z$

All $\hat{\theta}$'s have same s.e.$(\hat{\theta})$

standard error of $\hat{\theta}$: s.e.$(\hat{\theta}) = \sqrt{4/N}\,\hat{\sigma}$

t-statistic: $\hat{\theta}/\text{s.e.}(\hat{\theta})$

where σ^2 = variance of an observation.

❖ **Reading**: textbook, 4.3

Using Regression Analysis to Compute Factorial Effects

Design matrix

+ model

+ sum codings

Model matrix

treatment codings

cf.

model containing all factorial effects

- Consider the 2^3 design for factors A, B and C, whose columns are denoted by $\mathbf{x}_A$, $\mathbf{x}_B$ and $\mathbf{x}_C$ (= 1 or −1). ME codings
- The interactions AB, AC, BC, ABC are then equal to

$$\mathbf{x}_{AB} = \mathbf{x}_A\mathbf{x}_B,\ \mathbf{x}_{AC} = \mathbf{x}_A\mathbf{x}_C,\ \mathbf{x}_{BC} = \mathbf{x}_B\mathbf{x}_C,\ \mathbf{x}_{ABC} = \mathbf{x}_A\mathbf{x}_B\mathbf{x}_C$$

(see Table 3, LNp.5-10).

- Use the regression model (i = ith observation; j = jth effect)

matrix form

$Z = X\beta + \varepsilon$

model matrix

$\varepsilon \sim N(0, \sigma^2 I)$

functional form

$$z_i = \beta_0 + \sum_{j=1}^{\overset{7=8-1}{7}} \beta_j x_{ij} + \varepsilon_i,$$

$= \beta_0 + \beta_A x_A + \beta_B x_B + \beta_C x_C + \beta_{AB} x_A x_B + \beta_{AC} x_A x_C + \beta_{BC} x_B x_C + \beta_{ABC} x_A x_B x_C + \varepsilon$

- The regression (i.e., least squares) estimator of β_j is

$$\hat{\beta}_j = \frac{1}{1-(-1)}\left(\bar{z}(x_{ij}=+1) - \bar{z}(x_{ij}=-1)\right)$$

$$= \frac{1}{2}\,(\text{factorial effect of variable } x_j)$$

overall average

$\bar{z}(x_{A-})$ $\bar{z}(x_{A+})$

ME(A) $\hat{\beta}_A$

Model Matrix for 2^3 Design

$\hat{\beta} = (X^T X)^{-1} X^T Z$

$(X^T X)^{-1} = \frac{1}{2^k} I$

$X^T Z = \begin{bmatrix} \sum z_i \\ \sum z(x_{A+}) - \sum z(x_{A-}) \\ \vdots \end{bmatrix}$ e.g.

Table 3: Design Matrix and Model Matrix for 2^3 Design

μ	A	B	C	$\mathbf{1}$	$\mathbf{x}_A$	$\mathbf{x}_B$	$\mathbf{x}_C$	$\mathbf{x}_{AB}$	$\mathbf{x}_{AC}$	$\mathbf{x}_{BC}$	$\mathbf{x}_{ABC}$	z
$E(z_1)=\mu_{---}$	−	−	−	+	−	−	−	+	+	+	−	z_1
$E(z_2)=\mu_{--+}$	−	−	+	+	−	−	+	+	−	−	+	z_2
	−	+	−	+	−	+	−	−	+	−	+	z_3
•	−	+	+	+	−	+	+	−	−	+	−	z_4
•	+	−	−	+	+	−	−	−	−	+	+	z_5
•	+	−	+	+	+	−	+	−	+	−	−	z_6
	+	+	−	+	+	+	−	+	−	−	−	z_7
$E(z_8)=\mu_{+++}$	+	+	+	+	+	+	+	+	+	+	+	z_8

$\hat{\beta}_A = \frac{1}{8}\left[\sum z(x_{A+}) - \sum z(x_{A-})\right]$

$= \frac{1}{2}\left[\bar{z}(x_{A+}) - \bar{z}(x_{A-})\right]$

$= \frac{1}{2}\,\mathrm{ME}(A)$

model matrix X: a $2^k \times 2^k$ matrix whose columns are orthogonal and $X^T X = 2^k I$

$E(Z) = \mu = X\beta$

$\beta = X^{-1}\mu = \frac{1}{2^k} X^T \mu$

e.g. $\beta_A = \frac{1}{8}\left[\sum \mu(x_{A+}) - \sum \mu(x_{A-})\right]$

$= \frac{1}{2}\left[\bar{\mu}(x_{A+}) - \bar{\mu}(x_{A-})\right]$

$= \frac{1}{2}\,\mathrm{ME}(A)$