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# The inverse problem of bimorph mirror tuning on a beamline

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One of the challenges of tuning bimorph mirrors with many electrodes is that the calculated focusing voltages can be different by more than the safety limit (such as 500 V for the mirrors used at 17-ID at the Advanced Photon Source) between adjacent electrodes. A study of this problem at 17-ID revealed that the inverse problem of the tuning *in situ*, using X-rays, became ill-conditioned when the number of electrodes was large and the calculated focusing voltages were contaminated with measurement errors. Increasing the number of beamlets during the tuning could reduce the matrix condition number in the problem, but obtaining voltages with variation below the safety limit was still not always guaranteed and multiple iterations of tuning were often required. Applying Tikhonov regularization and using the L-curve criterion for the determination of the regularization parameter made it straightforward to obtain focusing voltages with well behaved variations. Some characteristics of the tuning results obtained using Tikhonov regularization are given in this paper.

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**Keywords: bimorph mirror; Tikhonov regularization; X-ray optics; inverse problem.**

## 1. Introduction

Multi-segmented bimorph mirrors using multiple 150 mm-long segments of piezoelectric ceramic (also called PZT) plates, with typically two or four and even eight electrodes per plate, have been developed and used for more than a decade at synchrotron beamlines (Signorato, 1998; Signorato & Ishikawa, 2001), with the capability of correcting the mirror shape down to the dimensions covered by each electrode, thus suppressing low-frequency mirror errors (Signorato *et al.*, 2001, 2004). They also have the potential to adaptively change their profiles for the so-called wavefront correction (Kimura *et al.*, 2009). To achieve the best result, each mirror has to be tuned, either in a metrology laboratory with such tools as a long trace profiler (LTP) or nanometre optical metrology (Siewert *et al.*, 2004; Alcock *et al.*, 2010; Sutter *et al.*, 2011), or at an X-ray beamline, using position measurement of many X-ray 'beamlets' (pencil beams) reflected from the mirror. Such tuning has also been called optimization or adaptive correction, and was introduced a decade ago (Signorato, 1998; Signorato *et al.*, 1998, 2001; Hignette *et al.*, 1997), based on the assumption of a linear relationship between the driving voltage on each electrode on a PZT plate and the induced curvature along the mirror. The calculation of the driving voltages for focusing becomes a typical discrete inverse problem mathematically. The number of electrodes in each bimorph mirror was only around three to five when this method was initially used for offline optimization in a metrology laboratory.

Owing to the fast development of technology, bimorph mirrors with as many as 16 electrodes are commonly used at synchrotron beamlines nowadays, and some mirrors have even more electrodes. The increased number of electrodes in the mirror increases the power of the shape correction. However, it also brings new challenges to *in situ* tuning with X-rays, as will be explained in this paper.

At the Advanced Photon Source (APS), the IMCA-CAT (Industrial Macromolecular Crystallography Association Collaboration Team) undulator beamline at sector 17 (17-ID) was recently upgraded, introducing a set of bimorph Kirkpatrick–Baez (KB) mirrors (supplied by Bruker ASC GmbH) with focal/source distances of 4.74 m/57.16 m [horizontal focusing mirror (HFM)] and 5.68 m/56.22 m [vertical focusing mirror (VFM)], and with demagnifications of 12 and 9.9, respectively. With fixed incident angles of 3 mrad and lengths of 1.05 m (HFM) and 0.6 m (VFM), these mirrors are long enough to accept the full undulator beam, which is about 1.7 mm (H) by 0.8 mm (V) FWHM at the mirror locations. There are four sets of the 150 mm-long PZT plates, each with four driving electrodes, inside the VFM, and there are seven sets of PZT plates, each with two driving electrodes with the exception of the central plate that has four electrodes, inside the HFM. So, there are 16 electrodes within each mirror. For the safety and integrity of the mirrors, the maximal allowable difference of voltages between any two adjacent electrodes is limited to 500 V. During the mirror tuning with X-rays on the beamline, however, it was not always straightforward to obtain a set of focusing voltages meeting this safety requirement, and generally multiple iterations of tuning were needed. We then

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found out that, even though a lot of attention was paid to the measurement accuracy, the matrix of the inverse problem of the correction became very ill-conditioned when the number of electrodes became large, such as 16. The calculated values of focusing voltages were then easily contaminated by measurement errors (or noise), even though such errors could be very small.

In order to make the inverse problem less ill-conditioned, we tried to improve the effective rank of the matrix in the inverse problem by using fewer independently powered electrodes and/or a larger number of beamlets along the mirror. This did reduce the variation of the calculated voltages, but keeping the maximal difference between adjacent electrodes below 500 V was still not always guaranteed.

A mathematical method, called Tikhonov regularization (Tikhonov & Arsenin, 1977), initially proposed to solve the so-called ill-posed inverse problem, has been successfully used in recent decades to solve many ill-conditioned problems in various scientific fields (*e.g.* Svergun, 1991; Ng *et al.*, 1999; Ying *et al.*, 2004). When this method was applied to the bimorph mirror tuning at IMCA-CAT, focusing voltages with well controlled fluctuation between electrodes were reliably achieved, and there was no need for multiple iterations of tuning. In other words, the Tikhonov regularization made it straightforward to converge to a satisfactory result for tuning of bimorph mirrors with a large number of electrodes.

This paper explains the challenges of directly solving the inverse problem of *in situ* mirror tuning with X-rays, describes our attempt to improve the solution stability of the inverse problem by increasing the number of beamlets, and finally gives a description of tuning using Tikhonov regularization and the characteristics of the results obtained with the regularization.

## 2. Errors in the inverse problem of bimorph mirror tuning

### 2.1. Brief description of bimorph mirror adaptive correction on a beamline with X-rays

For the reader's convenience, the widely used procedure of bimorph mirror tuning (or optimization, adaptive correction) on a beamline, introduced by Signorato *et al.* (Signorato, 1998; Signorato *et al.*, 1998, 2001), is briefly explained here. To calibrate the linear coefficients connecting the applied voltage on each electrode to the figure deformation along the mirror, the center of mass (COM) of each beamlet reflected from a section of mirror covered by each electrode is measured at the sample location (or any expected focusing location). For a mirror of $M$ electrodes, a minimal number of $M$ beamlet positions (or profile scans) at the sample location are normally measured. Such a measurement of $M$ beamlets normally starts with all the electrodes powered with the same voltage, and a roughly focused X-ray beam. Then the measurement of $M$ beamlet profiles is repeated after fixed interval voltage changes on each electrode. With $M(M + 1)$ position measurements of the beamlets at the sample location, a matrix $A \in R^{M\times M}$ is obtained and the target voltages on the $M$ electrodes needed for focusing, represented by a vector $x$, will be the solution of the following linear system,

$$Ax = b, \tag{1}$$

where $b$ is a vector of position differences of all the beamlets relative to the focal position. If the number of beamlets is not exactly the same as the number of electrodes, then $A \in R^{M\times N}$, $x \in R^N$, $b \in R^M$ (where $M$ and $N$ are the number of beamlets and electrodes, respectively). The singular value decomposition algorithm has been commonly used to find the solution of (1). Such adaptive mirror tuning on a beamline also corrects the perturbations on the incoming beam wavefront introduced by upstream optics.

### 2.2. Obtaining correction voltages by directly solving the inverse problem at 17-ID

At 17-ID the bimorph mirrors were designed to focus with negative voltages. According to the off-line characterization of the mirrors using the APS LTP, the HFM is pre-shaped with a cylindrical bending radius of 4.19 km and the VFM with a radius of 4.65 km, when the mirrors are not powered. The HFM RMS slope errors after cylindrical curvature subtraction are 1.37 µrad, with a peak-to-valley error of 10.14 µrad. The VFM RMS slope errors are 1.46 µrad, with a peak-to-valley error of 6.77 µrad. Sixteen beamlets were used; each of them was reflected by one section of the mirror corresponding to one electrode. Between each round of 16 profile measurements, the voltage of one electrode was shifted by −50 V. To minimize the time needed for the calibration, the beamlet profiles were often recorded using a CoolSnap camera with 5× objective and a YAG crystal of 1 µm-thick doped cerium. The resolution of this camera system was about 10 µm FWHM, tested with a 10 µm-diameter pinhole in front of the YAG crystal. While the beam size measurement was affected by the camera resolution (or point spread function), the measurement accuracy of the COM of the beamlets was mainly affected by the pixel size, which was 1.29 µm with the 5× objective, *i.e.* quite small. Some irregularities of the beamlet profiles (such as long tails on one side) affected the accuracy of the COM measurements of the main part of the beamlets, thus introducing some errors in both $A$ and $b$ in (1). More importantly, any potential beamline overall drift during tuning could also affect the accuracy of measurement. A 10 µm-diameter pinhole and a set of ∼6 µm opening slits were also used for beamlet COM measurement and cross checking.

By solving (1) using the calibrated 16 × 16 matrix $A$, we would normally obtained a voltage vector $x$ with variation between adjacent electrodes larger than the 500 V safety limit. Since the purpose of the tuning was to focus the beam while the exact transverse location of the focal point could be flexible (and adjustable by fine tweaking of mirror angles), we can introduce another variable $b_0$ in (1), making it into an underdetermined linear system with 17 unknowns,

$$Ax + b_0 = b, \tag{2}$$

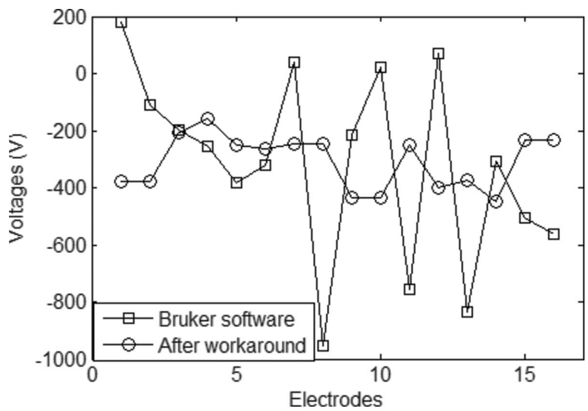


**Figure 1**
The squares show the voltages obtained using the software tool provided by the KB supplier Bruker-ASC using the HFM tuning data with 16 beamlets and 16 independently powered electrodes, where the safety limit of 500 V maximal difference between adjacent electrodes could not be satisfied. The circles show the voltages eventually achieved by workarounds, as explained in text.

from which the solution of both $x$ and $b_0$ can be found. When such an underdetermined system was solved using singular value decomposition (SVD), a solution with a minimal norm of $(x, b_0)$ was selected, with $x$ generally better than that given by the fully determined system in (1), in the sense of smaller fluctuations. Even so, the variation of the voltages was generally too large to be useful (we normally used the *ACM* software tool supplied by Bruker-ASC for the calculations, which can take the beamlet COM measurement data as the input and solve the inverse problem using a SVD algorithm), with a typical result shown by the squares in Fig. 1.

Several workarounds were used to obtain sets of voltages with variations less than the safety limit. For both the HFM and VFM, because of their large acceptance compared with the beam dimensions, the X-ray flux near the ends of the mirrors was low, therefore the two adjacent electrodes at each end of the mirrors could be supplied with the same voltages. We also combined the other electrodes into groups with mostly two electrodes per group; in this case the mirrors were used as if they had less than 16 electrodes and the obtained voltages normally had much lower fluctuations between any adjacent electrode groups. After such initial tuning with a small number of groups of electrodes, we repeated the tuning with more electrodes being powered independently, starting from previously tuned voltages. At the end of each tuning cycle the voltages on all the electrodes were also simultaneously shifted in small steps (such as $\pm 20$ V) while the changes of spot size at the sample location were monitored to search for the best focusing condition. Eventually the X-ray beam was focused with good symmetric profiles by a set of voltages shown by circles in Fig. 1.

### 2.3. Condition number of the matrix and calibration with more beamlets

For the inverse problem given by (1), the accuracy of the solution is related to the accuracy of matrix $A$ and vector $b$ by (*e.g.* Cheney & Kincaid, 2008)

**Table 1**
The decrease of condition numbers if tuning was performed with 16 beamlets but fewer electrodes.

| | Number of electrodes | | |
|---|---|---|---|
| | 7 | 14 | 16 |
| Data set 1 | 13 | 264 | 1377 |
| Data set 2 | 17 | 158 | 367 |
| Data set 3 | 54 | 731 | 907 |

$$\begin{aligned}
&\|\delta x\|/\|x\| \le \operatorname{cond}(A)/[1 - \operatorname{cond}(A)\|\delta A\|/\|A\|] \\
&\qquad \times (\|\delta b\|/\|b\| + \|\delta A\|/A) \qquad \text{or} \\
&\|\delta x\|/\|x\| \le \operatorname{cond}(A)\|\delta b\|/\|b\| \qquad \text{when } \delta\|A\| = 0, \text{ and} \\
&\|\delta x\|/\|x\| \le \operatorname{cond}(A)\|\delta A\|/\|A\| \qquad \text{when } \delta\|b\| = 0 \text{ and} \\
&\qquad\qquad \|\delta A\|/\|A\| \text{ is small,}
\end{aligned}$$

where $\operatorname{cond}(A) = \|A\| \cdot \|A\|^{-1} = \sigma_{\max}(A)/\sigma_{\min}(A)$ is the so-called 'condition number', determined by the ratio of maximal to minimal singular values, $\sigma_{\max}(A)$ and $\sigma_{\min}(A)$. A linear system with a very large condition number is called an ill-conditioned problem (or discrete ill-posed problem), and the solution can be highly contaminated by small errors in either $A$ or $b$. The last column in Table 1 includes some examples of condition numbers of our bimorph mirror correction matrix when the calibrations were carried out with 16 independently powered electrodes and 16 beamlets, with beamlet COMs in units of micrometers and voltages in units of volts. These large condition numbers explain the large variations of the calculated voltages when the problem was solved directly.

The large condition number of the matrix is normally related to the so-called rank-deficiency problem (Hansen, 1998), *i.e.* the number of columns of $A$ that, with respect to some error level, are linearly independent, is less than the number of positive singular values calculated mathematically. This could be caused by some degree of correlation among the COMs of the beamlets (*i.e.* the deformations along the mirror) measured between the voltage change on an electrode.

Two workarounds were initially tested at 17-ID to reduce the condition number, both based on a reduction of the number of independently powered electrodes. When we performed our very first calibration of the bimorph mirrors, the 16 electrodes of each mirror were grouped into seven groups and used as if there were only seven independent electrodes, and only seven beamlets from seven different sections of the mirror were used. This tuning ended up with sets of focusing voltages with variations within the 500 V limit. In this case the condition numbers of the matrices were around 260 (HFM) and 400 (VFM), apparently smaller than the average for the case of 16 electrodes.

Another way of reducing the number of independently powered electrodes was, after the measurement was made with 16 beamlets and 16 independent electrodes, only part of the measurement data were used in such a way as if the mirror had less than 16 electrodes but was measured with 16 beamlets, *i.e.* $A \in R^{M \times N}$, $x \in R^N$, $b \in R^M$, where $M = 16$, but $N < 16$ (such as $N = 7$ or 14 in Table 1). Keeping $M > N$ helped to

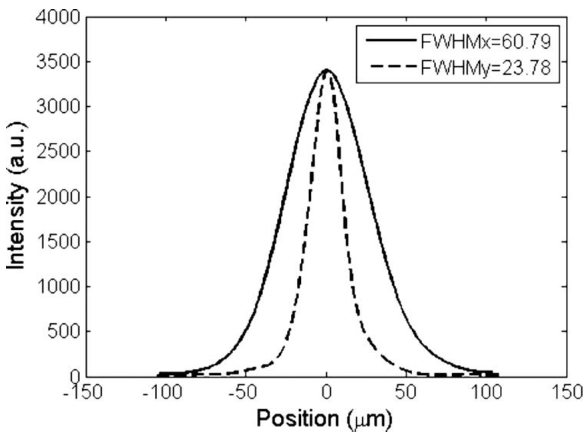


**Figure 2**
Minimal focal spot achieved on 17-ID so far, which corresponds to RMS slope errors of 1.26 μrad for the HFM and 0.89 μrad for the VFM.

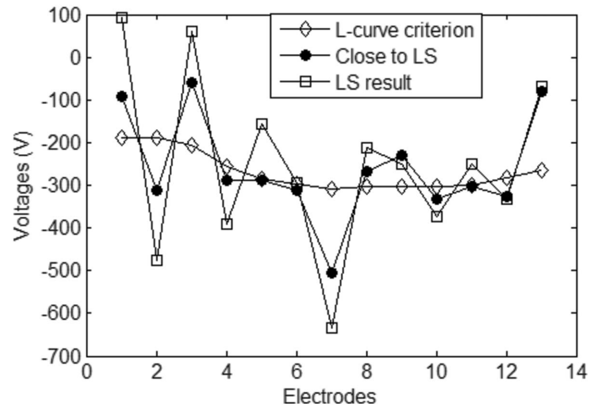


**Figure 3**
Calculated HFM focusing voltages using oversampled data measured with 13 independently powered electrodes (after blocking the beam tails on the mirror ends) and 21 beamlets, obtained by solving the inverse problem directly (squares, least-squares algorithm); using Tikhonov regularization with the L-curve criterion (diamonds) and with the regularization parameter shown by a circle in Fig. 8 (solid circles, with residual norm closer to the least-squares results).

reduce the matrix condition number, as shown in Table 1, and often a set of useful focusing voltages could be achieved when $N$ was small enough. When $N < M$, equation (1) becomes an overdetermined system with redundant data, which perhaps was helpful for increasing the effective rank, also called the numerical rank (Hansen, 1998) or pseudorank (Hanson, 1971), of the matrix. With this workaround, plus some tweaking of the voltages on all the electrodes after tuning and multiple iterations of tuning, the best focusing on record in the last two years, 61 μm (H) × 24 μm (V), was achieved (Fig. 2), measured using a CoolSnap camera (after spatial resolution deconvolution) and verified with ∼6 μm opening slit scans. The equivalent RMS slope errors of the mirrors were about 1.26 μrad (H) and 0.89 μrad (V) for this focal spot size. However, these workarounds of achieving applicable voltages by reducing the number of electrodes limited the full potential of using all the electrodes independently.

For the HFM, we tried further to use each electrode independently but to reduce the beamlet size from reflecting from one full electrode section to reflecting from half this size; therefore the number of beamlets could be increased to 32. However, it would take a lot of time to make the 17 × 32 measurements of the beamlet profiles (COMs). To shorten the calibration time (and also to reduce the chance of the beamline optics drifting during the calibration) we blocked the incident beam tails in front of the mirror and used only 13 electrodes for independent adjustment, and 21 beamlets (because in the middle of the HFM there are four electrodes having half the length of the remaining electrodes, therefore each beamlet for these four locations still covered a whole electrode area). The condition number of the matrix was reduced to 31 and the variations of the calculated voltages were smaller than the solutions using 16 electrodes and 16 beamlets. Unfortunately there were still occurrences of differences of slightly larger than 500 V between adjacent electrodes (such as around electrode #2, as shown by the squares in Fig. 3).

In short, *in situ* bimorph mirror tuning could become an ill-conditioned inverse problem of a fully determined system when the number of electrodes becomes large. Oversampling with reduced beamlet size to make it into an overdetermined linear system was effective in terms of reducing the condition number and finding voltages with less variation, but there was no guarantee that the results could always be good enough and within the safety limit. Multiple iterations of tuning were needed. Meanwhile, too much oversampling on a beamline takes a longer time and therefore could be more sensitive to the overall beamline stability.

## 3. Bimorph mirror tuning with Tikhonov regularization

### 3.1. Implementation of Tikhonov regularization to the mirror tuning

Tikhonov regularization is probably the most popular method used to solve ill-posed problems and ill-conditioned problems (Groetsch, 1984; Hansen, 1998). The basic idea of this method is to introduce a physically reasonable confinement to equation (1), and replace the inverse problem by finding the vector $x$ that minimizes the functional

$$\|Ax-b\|^2+\lambda^2\|Lx\|^2, \tag{3}$$

where $L$ is a discrete operator, $\|Lx\|$ is the regularization incorporated to stabilize the solution, and the regularization parameter $\lambda$ is used to balance the residual norm $\|Ax-b\|$ and the regularization norm $\|Lx\|$. For bimorph mirror tuning, a reasonable assumption (and also a practical requirement) for focusing voltages would be that there should be no large variations of the voltages between adjacent electrodes; therefore a discrete derivative operator was used for $L$. Finding the right regularization parameter $\lambda$ is a major part of using Tikhonov regularization. A too large regularization parameter will make the solution over-regularized with a too large residual error; on the other hand, a too small regularization parameter will make the solution highly contaminated by measurement errors. The so-called L-curve criterion (Lawson & Hanson, 1974; Hansen, 1992) has been successfully

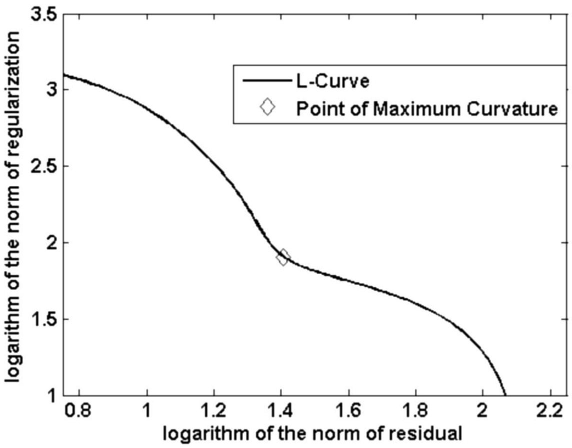


**Figure 4**
The L-curve applied to the mirror tuning on 17-ID. The selection of λ for the solution was determined by the location of the maximum curvature on the curve, as shown by the diamond, and the corresponding solution is given in Fig. 5 by diamonds.

used to find the appropriate value of λ for many discrete ill-conditioned problems (Hansen & O'Leary, 1993) even though it has limitations for infinite-dimensional problems (Hanke, 1996). An advantage of using the L-curve criterion is that no prior information about measurement errors is needed, and the balance between the residual norm and the regularization norm can be visualized in the L-shaped curve. For a plot of the L-shaped curve of $\log(\|Ax - b\|)$ *versus* $\log(\|Lx\|)$, obtained using

$$x = \arg\min_{x \in R^N} \left(\|Ax - b\|^2 + \lambda^2 \|Lx\|^2\right) \qquad (4)$$

for all valid values of λ, the best selection of the regularization parameter corresponds to the corner of this L-curve (where the L-curve has the maximum curvature), as shown in Fig. 4. The vector $x$ at the corner of this L-curve is selected as the solution to the linear system of equation (1) under regularization of $\|Lx\|$ (for mathematical details, please refer to, for example, Tikhonov & Arsenin, 1977; Hansen & O'Leary, 1993; Hansen, 1992; Van Loan, 1976). In Fig. 4, when $\|Ax - b\|$ approaches zero, $\|Lx\|$ represents the degree of voltage variation when (1) is fully satisfied; when $\|Lx\|$ approaches zero, $\|Ax - b\|$ represents the minimal focusing error when the same voltage is applied to all electrodes. The λ value at the corner of this L-curve represents the best balance of the two norms in (3), from where a slight decrease of any norm will cause an unfavorably large increase of another norm.

The diamonds in Fig. 5 represent the voltages calculated with Tikhonov regularization using the tuning data of the HFM measured with 16 independent electrodes and 16 beamlets, and this set of voltages gave favorable focusing with a FWHM of 66 μm. There was almost no voltage fluctuation along the mirror, with the absolute value gradually increasing from electrode #1 (at the upstream end of the mirror) to electrode #16 (at the downstream end of the mirror). Recalling that the IMCA-CAT HFM is rather long (1.05 m) and is located only 4.74 m from the sample (measured from the mirror center), the gradual change of the voltage in Fig. 5

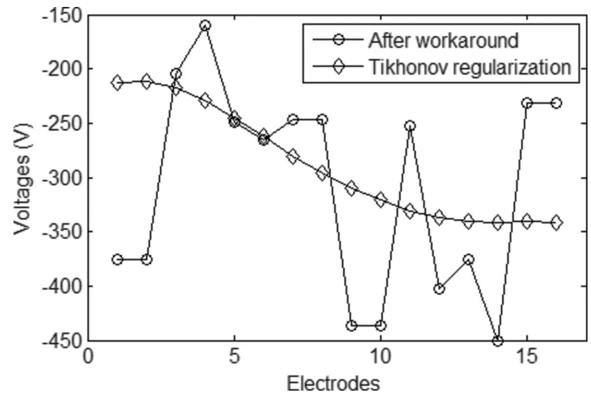


**Figure 5**
Comparison of the focusing voltages obtained by using Tikhonov regularization (diamonds) and the workaround approach (circles, the same results as shown in Fig. 1 with a different scale for the vertical axis).

represents the elliptical bending of this mirror as the mirror shape with all electrodes at the same voltage is basically cylindrical, as given by the mechanical polishing.

### 3.2. Multiple iterations of tuning with Tikhonov regularization, and a solution with smaller residual norm than that suggested by the L-curve criterion

When the correction voltage was calculated directly using (1) (and we normally used the software tool provided by Bruker-ASC for such calculation), it was often necessary to have more than one iteration of the tuning, *i.e.* more measurements on top of a set of focusing voltages obtained from previous tuning, for better focusing. To find out whether such a multiple-iteration technique was needed with Tikhonov regularization, and whether or not the regularization parameter λ given at the L-curve corner was actually the best choice, we carried out another round of measurements of all beamlet COMs after applying to the mirror the voltages previously obtained with Tikhonov regularization, and there were indeed differences among the COMs of these beamlets which meant there were still focusing errors between different sections of the mirror. Such focusing errors were used as the vector $b$ in (3) [and (4)], and another round of calculations with Tikhonov regularization was performed, with the L-curve and its 'corner' shown in Fig. 6. The fact that the corner of the L-curve was very close to its right-hand end meant that the new solution would not significantly reduce the residual norm, verified by its spot-size measurement of 67.2 μm (see the λ = 1.151 column in Table 2), which was close to the 66 μm obtained from the first round of tuning. Several different values of the regularization parameter λ with smaller residual norms along the L-curve were also selected (Fig. 6), with the corresponding sets of voltages given in Fig. 7, which would give better focusing if the influence of measurement errors was negligible, but they ended up with poorer focusing results as shown in Table 2. So, in this example, the Tikhonov regularization (together with the L-curve criterion) not only gave us a set of voltages with very small variation of voltages from electrode to electrode, but it also filtered out the noise caused by measurement errors.

**Table 2**
Measured HFM focal sizes using different sets of voltages (Fig. 7) obtained by choosing different λ along the L-curve (Fig. 6), for tuning without oversampling.

| | λ | | | | | |
|---|---|---|---|---|---|---|
| | 1.151 | 0.154 | 0.061 | 0.035 | 0.021 | 0.012 |
| $\|\|Ax - b\|\|$ (μm) | 39.34 | 34.10 | 28.85 | 23.60 | 18.36 | 13.11 |
| FWHM (μm) | 67.2 | 70.8 | 73.0 | 73.6 | 74.5 | 76.1 |

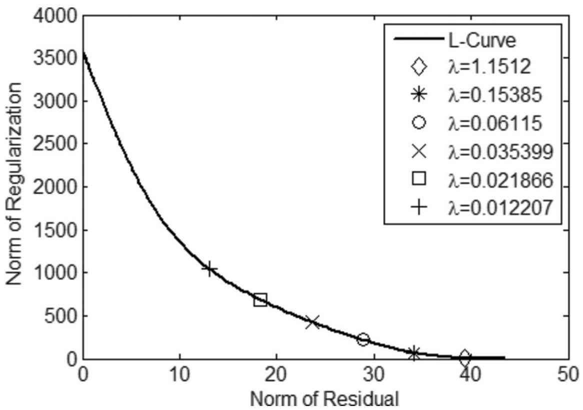


**Figure 6**
The L-curve of the second iteration of tuning after the mirror was applied with voltages given by Tikhonov regularization, on a linear scale. The diamond shows the point of maximum curvature (when plotted on a log–log scale as in Fig. 4), which is very close to the right-hand end of the curve. Five different regularization parameters (with decreased residual norms) along the L-curve were chosen with the corresponding voltages given in Fig. 7.

### 3.3. Tikhonov regularization for much oversampled data (overdetermined system)

Tikhonov regularization was also applied to the HFM tuning with beamlet number $M = 21$ and electrode number $N = 13$, with its L-curve shown in Fig. 8, plotted on a linear scale. The diamond represents the corner of the L-curve (the point of maximum curvature when plotted on a log–log scale), and the circle was another point arbitrarily selected on the L-curve that gave a very small residual norm and also a set of voltages within the safety limit of variations, as shown by solid circles in Fig. 3. The focusing spots generated by both sets of voltages were measured with very similar results, as shown in Fig. 9, suggesting that the set of voltages supposed for much smaller residual norm gave only slightly smaller focal size. So, in this example, the regularization together with the L-curve criterion still mostly filtered out the measurement noise (therefore significantly reducing voltage variations) and gave us a very satisfactory solution; meanwhile the regularization also filtered out some variations of voltages needed for slightly better focusing. Such information of 'necessary' variations mixed with measurement errors was difficult to distinguish without specific information about the measurement errors.

It is worthwhile mentioning that the smallest HFM focal spot achieved using regularization at 17-ID was 63 μm, slightly larger than the 61 μm record achieved by workaround (which was not reproducible by the time that the mirror was tuned by regularization).

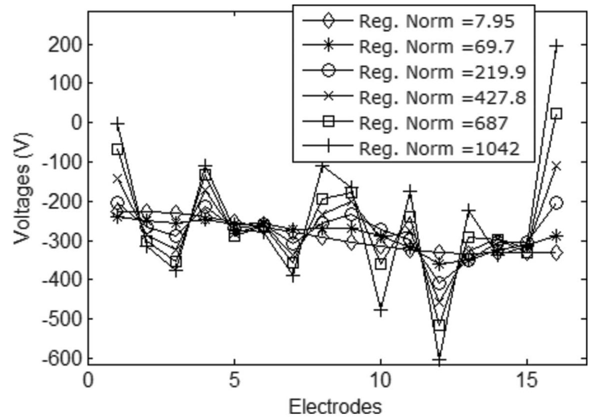


**Figure 7**
The gradual increase of voltage variations between electrodes as the regularization parameter and residual norms (shown in Fig. 6) decrease. The focal sizes using these sets of voltages are given in Table 2.

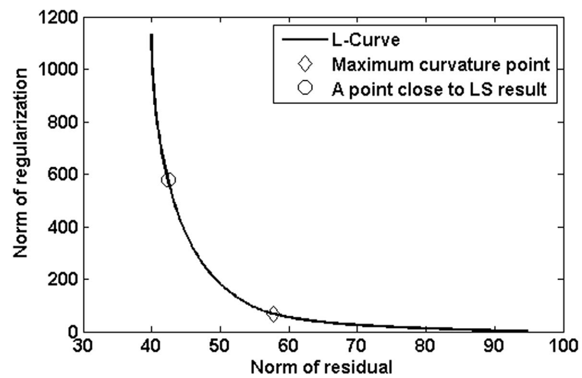


**Figure 8**
The L-curve using the oversampled data measured with reduced beamlet size for HFM tuning, with the diamond representing the 'corner' of the L-curve on a log–log scale and the circle representing a point of reduced regularization parameter with the residual norm close to the minimal achievable by the least-squares algorithm. The calculated voltages of these two points are shown in Fig. 3 by diamonds and solid circles, respectively.

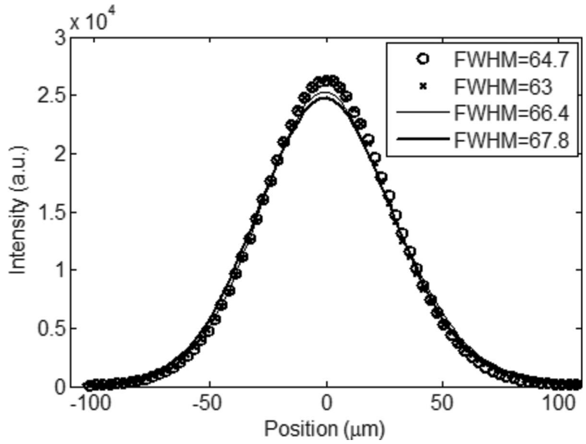


**Figure 9**
From top to bottom in the legend, the spot profiles focused with the voltages given by the regularization parameter at the 'corner' of the L-curve in Fig. 8; the circle at the L-curve in Fig. 8; voltages at the L-curve corner −15 V; voltages at L-curve corner +15 V.

### 3.4. Accuracy of mirror tuning with Tikhonov regularization

After applying to the mirror the voltages given by directly solving equation (1), it was common practice to tweak the voltages on all the electrodes simultaneously towards either the plus or minus direction to search for better potential focusing voltages. To tune the mirror by Tikhonov regularization, it was found that such a practice of tweaking was not necessary (given a beamline with stable optics). An example is shown in Fig. 9 where, after the mirror was powered with the voltages given by the Tikhonov regularization (the diamonds in Fig. 3), the voltages on all the electrodes were tweaked by 15 V towards both positive and negative directions, causing poorer focusing in both cases, though not by much.

### 3.5. Using Tikhonov regularization for 17-ID VFM tuning

Compared with the HFM at 17-ID, the VFM at 17-ID is further upstream from the sample with a larger focal distance of 5.68 m, and the mirror is also shorter, with a length of 600 mm. When Tikhonov regularization was implemented, the tuning results did not show a pattern of obvious elliptical bending. The benefit of using Tikhonov regularization (with regularization parameter $\lambda$ determined by the L-curve criterion) was that it guaranteed a set of voltages with smaller variations between electrodes (Fig. 10), satisfactory focusing (with FWHM of 26 µm), and no need for multiple iterations of tuning. The measured spot size was also slightly larger than the smallest size measured over the last couple years at 17-ID, which was about 24 µm, but it was not clear to us whether such a small difference was caused by some change of beamline optics condition or by some 'overfiltering' by the regularization, as shown in the case of HFM tuning with oversampled data.

## 4. Conclusions

As the number of electrodes in a bimorph mirror increases to as many as 16 or more nowadays, the inverse problem of the fully determined system of equation (1) becomes ill-conditioned and the results become highly sensitive to measurement errors and beamline overall drifts when the mirror is tuned *in situ* with X-rays. At 17-ID, oversampling with reduced beamlet size was very useful in the sense of reducing the condition number of the matrix, therefore obtaining the voltage set with less variation, but the achievement of a set of voltages within the limit of safety for elastic deformation of the mirror was never guaranteed. Multiple iterations of tuning were often used as a workaround to achieve good focusing.

By introducing extra confinement on the inverse problem using Tikhonov regularization, we were able to reliably achieve a set of focusing voltages with well contained variations. The L-curve criterion of choosing the regularization parameter was used because it does not require prior information about measurement errors and the results can be visually examined. The mirror tuning using Tikhonov regularization was straightforward in the sense that there was no need for multiple iterations of tuning and there was also no need for further tweaking of the voltages on the electrodes on top of the calculated voltages.

Under certain conditions, such as in our example of oversampling with smaller beamlet size where the condition number of the matrix also became small, the regularization imposed also filtered out some voltage variations needed for better focusing. So using Tikhonov regularization together with the L-curve criterion is a useful way to tune the mirror with satisfactory results, but it is not an automatic way to find the ultimate limit of a mirror's focusing potential.

In short, the regularization is not only useful for the case where people take short cuts by not taking many redundant measurements (which is often needed when calibration is performed at a beamline with X-rays), but it is also useful in a more general scope as well in the way that it guarantees a solution at any level of voltage variation you wish, for any number of data points. Redundant measurements give a small matrix condition number but do not always guarantee a set of focusing voltages with small variations.

As a brief discussion, if the measurement errors are quantitatively known, they could be used to better define the regularization parameter $\lambda$, for better results than using the L-curve criterion. In the end, the Tikhonov regularization can be considered as another kind of workaround when the inverse problem is ill-conditioned or the variation is just too large even if it is given accurately with a very small matrix condition number. It is always a good idea, if possible, to tune the mirror on a beamline in a way that makes the problem less ill-conditioned, such as using more beamlets with smaller beamlet size. Fast beamlet profile measurements by 'on-the-fly' continuous scan or any set-up on the beamline providing fast and accurate beam profile measurements will be very helpful. Finally, improvement of the quality of the mirror is also another important factor in reducing the relative variation of voltages between electrodes.

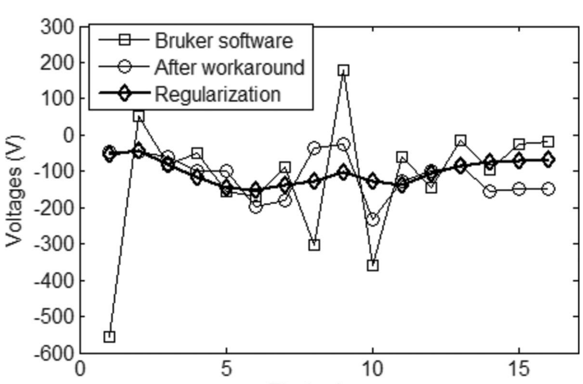


**Figure 10**
The VFM focusing voltages given by directly solving the inverse problem (with Bruker-ASC software, squares), after workaround (circles) and with Tikhonov regularization (diamonds).

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## References

Alcock, S. G., Sawhney, K. J. S., Scott, S., Pedersen, U., Walton, R., Siewert, F., Zeschke, T., Senf, F., Noll, T. & Lammert, H. (2010). *Nucl. Instrum. Methods Phys. Res. A*, **616**, 224–228.

Cheney, W. & Kincaid, D. (2008). *Numerical Mathematics and Computing*, 6th ed. Belmont: Brooks/Cole.

Groetsch, C. W. (1984). *The Theory of Tikhonov Regularization for Fredholm Equations of the First Kind.* Boston: Pitman.

Hanke, M. (1996). *BIT Numer. Math.* **36**, 287–301.

Hansen, P. C. (1992). *SIAM Rev.* **34**, 561–580.

Hansen, P. C. (1998). *Rank-Deficient and Discrete Ill-posed Problems: Numerical Aspects of Linear Inversion.* Philadelphia: Society for Industrial and Applied Mathematics.

Hansen, P. C. & O'Leary, D. P. (1993). *SIAM J. Sci. Comput.* **14**, 1487–1503.

Hanson, R. J. (1971). *SIAM J. Numer. Anal.* **8**, 616–622.

Hignette, O., Freund, A. & Chinchio, E. (1997). *Proc. SPIE*, **3152**, 188–199.

Kimura, T., Handa, S., Mimura, H., Yumoto, H., Yamakawa, D., Matsuyama, S., Inagaki, K., Sano, Y., Tamamsaku, K., Nishino, Y., Yabashi, M., Ishikawa, T. & Yamauchi, K. (2009). *Jpn. J. Appl. Phys.* **48**, 072503.

Lawson, C. L. & Hanson, R. J. (1974). *Solving Least Squares Problems.* Englewood Cliffs: Prentice-Hall.

Ng, M. K., Chan, R. H. & Tang, W. (1999). *SIAM J. Sci. Comput.* **21**, 851–866.

Siewert, F., Noll, T., Schlegel, T., Zeschke, T. & Lammert, H. (2004). *AIP Conf. Proc.* **705**, 847–850.

Signorato, R. (1998). *Proc. SPIE*, **3447**, 20–31.

Signorato, R., Carre, J.-F. & Ishikawa, T. (2001). *Proc. SPIE*, **4501**, 76–87.

Signorato, R., Hausermann, D., Somayazulu, M. & Carre, J.-F. (2004). *Proc. SPIE*, **5193**, 112–123.

Signorato, R., Hignette, O. & Goulon, J. (1998). *J. Synchrotron Rad.* **5**, 797–800.

Signorato, R. & Ishikawa, T. (2001). *Nucl. Instrum. Methods Phys. Res. A*, **467–468**, 271–274.

Sutter, J. P., Alcock, S. & Sawhney, K. (2011). *Diamond Light Source Proc.* **1**, e10.

Svergun, D. I. (1991). *J. Appl. Cryst.* **24**, 485–492.

Tikhonov, A. N. & Arsenin, V. Y. (1977). *Solutions of Ill-Posed Problems.* Washington: John Wiley and Sons.

Van Loan, C. F. (1976). *SIAM J. Numer. Anal.* **13**, 76–83.

Ying, L., Xu, D. & Liang, Z.-P. (2004). *Proceedings of the 26th Annual International Conference of the IEEE Engineering in Medicine and Biology Society (EMBS 2004)*, San Francisco, CA, USA. 1–5 September 2004, pp. 1056–1059.